When nA is 0:

=> fil cap

FILE 'CAPLUS' ENTERED AT 12:21:07 ON 24 DEC 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 24 Dec 2008 VOL 149 ISS 26 FILE LAST UPDATED: 23 Dec 2008 (20081223/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third guarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

VAR G2=H/17/18/20/22/24/26/29/32/34 NODE ATTRIBUTES: CONNECT IS E2 RC AT 1

CONNECT IS X4 RC AT 19 CONNECT IS X4 RC AT 25 CONNECT IS X4 RC AT 28

```
CONNECT IS X4 RC AT 31
CONNECT IS E1 RC AT 33
CONNECT IS X4 RC AT 35
CONNECT IS X4 RC AT 39
DEFAULT MLEVEL IS ATOM
GGCAT IS LOC UNS AT 17
GGCAT IS LOC
             SAT AT 19
GGCAT IS LOC
             SAT AT 25
GGCAT IS LOC SAT AT 28
GGCAT IS LOC SAT AT 31
GGCAT
      IS UNS AT 35
GGCAT IS LOC SAT AT 39
DEFAULT ECLEVEL IS LIMITED
```

GRAPH ATTRIBUTES: RSPEC 6 9

NUMBER OF NODES IS 42

STEREO ATTRIBUTES: NONE

L3 869 SEA FILE=REGISTRY SSS FUL L1 L7 STR

Page 2-A
VAR G2=H/17/18/20/22/24/26/29/32/34
VAR G3=0H/45/COOH/47/20/51/55/60/65/68/76/77
NODE ATTRIBUTES:
CONNECT 15 E2 RC AT 1
CONNECT 15 X4 RC AT 19

3

```
CONNECT IS X4 RC AT 25
CONNECT IS X4 RC AT 28
CONNECT IS X4 RC AT 31
CONNECT IS E1 RC AT 33
CONNECT IS X4 RC AT 35
CONNECT IS X4 RC AT 39
CONNECT IS E2 RC AT 73
CONNECT IS E2 RC AT 74
CONNECT IS E3 RC AT 76
DEFAULT MLEVEL IS ATOM
GGCAT IS LOC UNS AT 17
GGCAT IS LOC SAT AT 19
GGCAT
      IS LOC
             SAT
                  AT
                      2.5
GGCAT IS LOC SAT AT 28
GGCAT IS LOC SAT AT 31
GGCAT IS UNS AT 35
GGCAT IS LOC SAT AT 39
DEFAULT ECLEVEL IS LIMITED
```

GRAPH ATTRIBUTES: RSPEC 6 9

NUMBER OF NODES IS 78

STEREO ATTRIBUTES: NONE

L9 15 SEA FILE=REGISTRY SUB=L3 SSS FUL L7
L10 2 SEA FILE=CAPLUS SPE=ON ABB=ON PLU=ON L9

L12 STR

Page 2-A VAR G2=H/17/18/20/22/24/26/29/32/34

```
VAR G4=H/X/CN/NO2/45/46/48/49/NH2/52/55/COOH/57/61/63/64/66
NODE ATTRIBUTES:
CONNECT IS E2 RC AT
CONNECT IS X4 RC AT 19
CONNECT IS X4 RC AT 25
CONNECT IS X4 RC AT 28
CONNECT IS X4 RC AT 31
CONNECT IS E1 RC AT 33
CONNECT IS X4 RC AT 35
CONNECT IS X4 RC AT 39
CONNECT IS X4 RC AT 45
CONNECT IS X4 RC AT 47
CONNECT IS X4 RC AT 48
CONNECT IS X4 RC AT 50
CONNECT IS E1 RC AT 53
CONNECT IS E1 RC AT 54
CONNECT IS E1 RC AT 56
CONNECT IS X4 RC AT 59
CONNECT IS X4 RC AT 62
CONNECT IS X5 RC AT 63
CONNECT IS E2 RC AT 64
CONNECT IS X4 RC AT 65
CONNECT IS E2 RC AT 66
CONNECT IS X4 RC AT 67
DEFAULT MLEVEL IS ATOM
GGCAT IS LOC UNS AT 17
GGCAT IS LOC SAT AT 19
GGCAT IS LOC SAT AT 25
GGCAT IS LOC SAT AT 28
GGCAT IS LOC SAT AT 31
GGCAT IS UNS AT 35
GGCAT IS LOC SAT AT 39
GGCAT IS LOC AT 45
GGCAT IS LOC SAT AT 47
GGCAT IS SAT AT 48
GGCAT IS LOC SAT AT 50
GGCAT IS LOC SAT AT 53
GGCAT IS LOC SAT AT 54
GGCAT IS LOC SAT AT 56
GGCAT IS LOC SAT AT 59
GGCAT IS UNS AT 62
GGCAT IS UNS AT 63
GGCAT IS SAT AT 64
GGCAT IS UNS AT 65
GGCAT IS SAT AT 66
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RSPEC 6 9
NUMBER OF NODES IS 67
STEREO ATTRIBUTES: NONE
L14
           322 SEA FILE=REGISTRY SUB=L3 SSS FUL L12
            39 SEA FILE=CAPLUS SPE=ON ABB=ON PLU=ON L14
L15
            1 SEA FILE=CAPLUS SPE=ON ABB=ON PLU=ON L10 AND L15
L18
             2 SEA FILE=CAPLUS SPE=ON ABB=ON PLU=ON L17 OR L10
```

=> d 118 ibib abs hitstr tot

L18 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:612072 CAPLUS Full-text DOCUMENT NUMBER: 143:146661 TITLE: Hsp90 family protein inhibitor

INVENTOR(S): Kitamura, Yushi; Nara, Shinji; Nakagawa, Hiroshi; Nakatsu, Rieko; Nakashima, Takayuki; Soga, Shiro; Kajita, Jiro; Shiotsu, Yukimasa; Kanda, Yutaka

PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan

SOURCE: PCT Int. Appl., 311 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA	PATENT NO.					D	DATE		APPLICATION NO.					DATE			
WO	VO 2005063222				A1 20050714			WO 2004-JP19742					20041224				
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
		TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
		ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IS,	IT,	LT,	LU,	MC,	NL,	PL,	PT,
		RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,
		MR,	NE,	SN,	TD,	TG											
EP	EP 1704856				A1 20060927				EP 2004-808092					20041224			
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		IE,	SI,	LT,	FI,	RO,	CY,	TR,	BG,	CZ,	EE,	HU,	PL,	SK,	IS		
US	US 20070155813				A1 20070705					US 2006-584234				20060626			
PRIORIT	RIORITY APPLN. INFO.:									JP 2003-432776				A 20031226			
										WO 2	004-	JP19	742	1	vi 2	0041	224
OTHER S	THER SOURCE(S):						MARPAT 143:146661										

OT GI

A Hsp90 family protein inhibitor which contains as an active ingredient a AB benzene derivative represented by the following general formula (I), a prodrug thereof, or a pharmacol, acceptable salt of either.

860151-78-6P 860151-80-0P 860151-83-3P 860151-36-6P 860151-87-7P 860151-88-8P 860151-90-2P 860151-92-4P 860151-94-6P 860151-96-8P 860151-98-0P 860152-00-7P 860152-01-8P 860152-03-0P 860152-04-1P 860152-05-2P 860152-06-3P 360152-07-4P

```
860152-08-5P 860152-09-6P 860152-10-9P
860152-11-0P 860152-12-1P 860152-13-2P
260152-14-3P 860152-15-4P 860152-16-5P
860152-17-6P 860152-18-7P 860152-19-8P
860152-20-1P 860152-21-2P 860152-22-3P
860152-23-4P 860152-24-5P 860152-25-6P
860152-26-7P 860152-27-8P 860152-28-9P
860152-39-0P 860152-30-3P 860153-31-4P
860152-32-5P 860152-33-6P 860152-34-7P
860152-35-8P 860152-36-9P 860152-37-0P
860152-38-1P 860152-39-2P 860152-40-5P
860152-41-6P 860152-42-7P 860152-43-8P
860152-44-9P 860152-45-0P 860152-46-1P
960152-47-2P 860152-48-3P 860152-49-4P
860152-50-7P 860152-51-8P 860152-52-9P
860152-53-0P 860152-54-1P 860152-55-2P
860152-56-3P 860152-57-4P 860152-58-5P
860152-59-6P 860152-60-9P 860152-61-0P
860152-62-1P 860152-63-2P 860152-64-3P
860152-65-4P 860152-66-5P 860152-67-6P
860152-68-7P 860153-69-8P 860152-70-1P
860152-71-3P 860152-72-3P 860152-73-4P
860152-74-5P 860152-75-6P 860152-76-7P
960152-77-8F 860152-78-9F 860152-79-0F
860152-80-3P 860152-81-4P 860152-82-5P
860152-83-6P 860152-84-7P 360152-85-8P
860152-87-0P 860152-88-1P 860152-89-2P
860152-90-5P 860152-91-6P 860152-92-7P
860152-93-8P 860152-94-9P 860152-95-0P
860152-96-1P 860152-98-3P 860152-99-4P
860153-00-0P 860153-01-1P 860153-02-2P
860153-03-3P 860153-04-4P 860153-05-5P
860153-06-6P 860153-07-7P 860153-08-8P
960153-09-9P 860153-10-2P 860153-11-3P
860153-12-4P 860153-13-5P 860153-15-7P
860153-16-8P 860153-17-9P 860153-18-0P
860153-19-1P 860153-20-4P 860153-21-5P
860153-22-6P 860153-23-7P 860153-24-8P
860153-25-9P 860153-26-0P 860153-27-1P
860153-28-2P 860153-29-3P 860153-30-6P
860153-31-7P 860153-32-8P 860153-33-9P
860153-35-1P 860153-36-2P 860153-37-3P
860153-38-4P 860153-39-5P 860153-40-8P
860153-41-9P 860153-42-0P 860153-43-1P
860153-44-2P 860153-45-3P 860153-46-4P
860153-47-5P 860153-48-6P 860153-49-7P
860153-50-0P 860153-51-1P 860153-52-2P
860153-53-3P 860153-54-4P 860153-55-5P
860153-56-6P 860153-57-7P 860153-58-8P
860153-59-9P 860153-60-2P 860153-61-3P
860153-62-4P 860153-63-5P 860153-64-6P
860153-65-7P 860153-66-8P 860153-67-9P
860153-68-0P 860153-69-1P 860153-70-4P
960153-71-5P 860153-72-6P 860153-73-7P
860153-74-8P 860153-75-9P 860153-76-0P
860153-77-1P 860153-78-2P 860153-79-3P
860153-80-6P 860153-81-7P 860153-82-8P
860153-83-9P 860153-84-0P 860153-85-1P
860153-86-2P 860153-87-3P 860153-88-4P
860153-89-5P 860153-90-8P 860153-91-9P
```

860153-92-09 860152-93-1P 860153-93-2P 860153-97-5P 860153-98-69 860153-99-7P 860153-99-7P 860153-99-7P 860153-99-7P 860153-98-6P 860153-09-6P 860154-00-3P 860154-01-4P 860154-05-8P 860154-05-8P 860153-07-0P 860154-08-1P 860154-01-2P 860154-10-5P 860154-10-8P 860154-11-2P 860154-11-2P 860154-11-2P 860154-11-2P 860154-11-4P 860154-49-4P 860154-49-4-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(benzene derivs. as Hsp90 family protein inhibitors and antitumor agents)

RN 860151-78-6 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-, methyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{HO} & \overset{\circ}{\underset{\text{OH}}{\bigoplus}} \text{OMe} \end{array}$$

RN 860151-80-0 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-3'-(3-oxo-1-buten-1-yl)-, methyl ester (CA INDEX NAME)

RN 860151-83-3 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-3'-[(hydroxyimino)methyl]-,
 methyl ester (CA INDEX NAME)

RN 860151-86-6 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-3'-[(methoxyimino)methyl]-,
 methyl ester (CA INDEX NAME)

RN 860151-87-7 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-3'-(3-oxobutyl)-, methyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} \stackrel{\circ}{\underbrace{\hspace{1cm}}} \text{CH}_2 \\ \text{HO} \end{array} \qquad \begin{array}{c} \text{CH}_2 \text{--} \text{CH}_2 - \stackrel{\circ}{\underbrace{\hspace{1cm}}} \text{Me} \end{array}$$

RN 860151-88-8 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-2'-methoxy-, methyl ester
(CA INDEX NAME)

RN 860151-90-2 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 2'-chloro-4,6-dihydroxy-, methyl ester (CA INDEX NAME)

RN 860151-92-4 CAPLUS

CN [1,1'-Bipheny1]-2-acetic acid, 3'-acetyl-4,6-dihydroxy-, methyl ester (CA INDEX NAME)

RN 860151-94-6 CAPLUS

CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-N-[2-(dimethylamino)ethyl]-4,6dihydroxy- (CA INDEX NAME)

RN 860151-96-8 CAPLUS

CN [1,1'-Bipheny1]-2-acetic acid, 3-bromo-4,6-dihydroxy-, methyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{Ph} & \bigcap\limits_{\text{OH}} \text{CH}_2 - \bigcap\limits_{\text{C}} \text{OMe} \end{array}$$

RN 860151-98-0 CAPLUS

CN [1,1':3',1''-Terpheny1]-2'-acetic acid, 4',6'-dihydroxy-, methy1 ester
(9CI) (CA INDEX NAME)

RN 860152-00-7 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 3-bromo-4,6-dihydroxy- (CA INDEX NAME)

RN 860152-01-8 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-3-iodo-, methyl ester (CA INDEX NAME)

RN 860152-03-0 CAPLUS

CN [1,1'-Bipheny1]-2-acetic acid, 4,6-dihydroxy-3-(4-morpholinylmethyl)-,
 methyl ester (CA INDEX NAME)

- RN 860152-04-1 CAPLUS
- CN [1,1'-Biphenyl]-2,4-diol, 5-bromo-6-(hydroxymethyl)- (CA INDEX NAME)

- RN 860152-05-2 CAPLUS
- CN [1,1'-Bipheny1]-2-acetamide, N-[2-(acetylamino)ethy1]-3-bromo-4,6dihydroxy- (CA INDEX NAME)

HO
$$CH_2$$
 CH_2 CH_2 CH_2 CH_3 CH_4 CH_4 CH_5 CH_5

- RN 860152-06-3 CAPLUS
- CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N-(3-pyridinylmethyl)-(CA INDEX NAME)

- RN 860152-07-4 CAPLUS
- CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N-[1-(phenylmethyl)-4piperidinyl]- (CA INDEX NAME)

RN 860152-08-5 CAPLUS

- RN 860152-09-6 CAPLUS
- CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N-(2-methylpropyl)-(CA INDEX NAME)

- RN 860152-10-9 CAPLUS
- CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N-propyl- (CA INDEX NAME)

- RN 860152-11-0 CAPLUS
- CN [1,1'-Bipheny1]-2-acetamide, 3-bromo-4,6-dihydroxy-N-[3-(2-oxo-1pyrrolidiny1)propy1]- (CA INDEX NAME)

RN 860152-12-1 CAPLUS

CN [1,1'-Bipheny1]-2-acetamide, 3-bromo-4,6-dihydroxy-N-(2-methoxyethy1)(CA INDEX NAME)

RN 860152-13-2 CAPLUS

CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N-(phenylmethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{Br} & \overset{\circ}{\underset{\text{CH}_2}{\bigcap}} \text{CH}_2 - \overset{\circ}{\underset{\text{C}}{\bigcap}} \text{NH-CH}_2 - \text{Ph} \\ \\ \text{Ph} & \\ \end{array}$$

RN 860152-14-3 CAPLUS

CN [1,1'-Bipheny1]-2,4-dio1, 5-bromo-6-[(phenylmethoxy)methy1]- (CA INDEX NAME)

- RN 860152-15-4 CAPLUS
- CN [1,1'-Biphenyl]-2,4-diol, 5-bromo-6-(methoxymethyl)- (CA INDEX NAME)

- RN 860152-16-5 CAPLUS
- CN [1,1'-Biphenyl]-2,4-diol, 5-bromo-6-[(2-propen-1-yloxy)methyl]- (CA INDEX NAME)

- RN 860152-17-6 CAPLUS
- CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-N-[(2,4-dimethoxyphenyl)methyl]-4,6dihydroxy- (CA INDEX NAME)

- RN 860152-18-7 CAPLUS
- CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N-methyl-N-(phenylmethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{Br} & \overset{\circ}{\text{CH}_2} - \overset{\circ}{\text{Ne}} \\ \text{Ho} & \overset{\circ}{\text{Ne}} - \overset{\circ}{\text{CH}_2} - \overset{\circ}{\text{Ph}} \end{array}$$

RN 860152-19-8 CAPLUS

CN Ethanone, 2-(3-bromo-4,6-dihydroxy[1,1'-biphenyl]-2-yl)-1-[4-(phenylmethyl)-1-piperidinyl]- (CA INDEX NAME)

- RN 860152-20-1 CAPLUS
- CN Ethanone, 2-(3-bromo-4,6-dihydroxy[1,1'-biphenyl]-2-yl)-1-[4-(phenylmethyl)-1-piperazinyl]- (CA INDEX NAME)

- RN 860152-21-2 CAPLUS
- CN Ethanone, 2-(3-bromo-4,6-dihydroxy[1,1'-biphenyl]-2-yl)-1-(4-methyl-1piperazinyl)- (CA INDEX NAME)

- RN 860152-22-3 CAPLUS

- RN 860152-23-4 CAPLUS
- CN Ethanone, 2-(3-bromo-4,6-dihydroxy[1,1'-biphenyl]-2-yl)-1-(3,4-dihydro-

2(1H)-isoquinoliny1)- (CA INDEX NAME)

$$\bigcap_{h} \bigcap_{c} \bigcap_{cH2} \bigcap_{h} \bigcap_{cH} \bigcap_$$

RN 860152-24-5 CAPLUS

RN 860152-25-6 CAPLUS

CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N-methyl-N-propyl- (CA INDEX NAME)

RN 860152-26-7 CAPLUS

CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N-(2-methoxyethyl)-Nmethyl- (CA INDEX NAME)

$$\begin{array}{c} \text{Br} & \overset{\text{O}}{\longrightarrow} \text{Me} \\ \text{CH}_2 - \overset{\text{O}}{\longrightarrow} \text{H} - \text{CH}_2 - \text{CH}_2 - \text{OMe} \end{array}$$

RN 860152-27-8 CAPLUS

CN Benzonitrile, 2-[4-[2-(3-bromo-4,6-dihydroxy[1,1'-biphenyl]-2-yl)acetyl]-1-

piperazinyl]- (CA INDEX NAME)

RN 860152-28-9 CAPLUS

CN Ethanone, 2-(3-bromo-4,6-dihydroxy[1,1'-bipheny1]-2-y1)-1-[4-(3pyridinylmethyl)-1-piperaziny1]- (CA INDEX NAME)

$$\text{CH}_2 - \text{N} - \text{CH}_2 - \text{OI}$$

RN 860152-29-0 CAPLUS

CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy- (CA INDEX NAME)

RN 860152-30-3 CAPLUS

CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N-methyl- (CA INDEX NAME)

RN 860152-31-4 CAPLUS

CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N,N-dimethyl- (CA

INDEX NAME)

RN 860152-32-5 CAPLUS

CN [1,1'-Bipheny1]-2,4-diol, 5-bromo-6-(phenoxymethy1)- (CA INDEX NAME)

RN 860152-33-6 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 5-bromo-6-methyl- (CA INDEX NAME)

RN 860152-34-7 CAPLUS

CN [1,1'-Biphenyl]-2-carboxylic acid, 3-bromo-4,6-dihydroxy- (CA INDEX NAME)

RN 860152-35-8 CAPLUS

CN [1,1'-Biphenyl]-2-carboxylic acid, 3-bromo-4,6-dihydroxy-, methyl ester (CA INDEX NAME)

RN 860152-36-9 CAPLUS

CN [1,1'-Biphenyl]-2-carboxamide, 3-bromo-4,6-dihydroxy-N-methyl- (CA INDEX NAME)

RN 860152-37-0 CAPLUS

CN [1,1'-Biphenyl]-2-carboxamide, 3-bromo-4,6-dihydroxy-N,N-dimethyl- (CA INDEX NAME)

RN 860152-38-1 CAPLUS

CN [1,1'-Bipheny1]-2-carboxamide, 3-bromo-4,6-dihydroxy- (CA INDEX NAME)

RN 860152-39-2 CAPLUS

CN [1,1'-Bipheny1]-2-carboxamide, 3-bromo-4,6-dihydroxy-N-(phenylmethy1)-(CA INDEX NAME)

RN 860152-40-5 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 3-ethyl-4,6-dihydroxy-, methyl ester (CA INDEX NAME)

RN 860152-41-6 CAPLUS

CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N-(2-pyridinylmethyl)-(CA INDEX NAME)

RN 860152-42-7 CAPLUS

CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N-(4-pyridinylmethyl)-(CA INDEX NAME)

RN 860152-43-8 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 3-formyl-4,6-dihydroxy-, methyl ester (CA INDEX NAME)

RN 860152-44-9 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-3-methyl-, methyl ester (CA INDEX NAME)

RN 860152-45-0 CAPLUS

CN 1-Propanone, 1-(3-bromo-4,6-dihydroxy[1,1'-biphenyl]-2-yl)- (CA INDEX NAME)

RN 860152-46-1 CAPLUS

CN Methanone, (3-bromo-4,6-dihydroxy[1,1'-biphenyl]-2-yl)phenyl- (CA INDEX NAME)

RN 860152-47-2 CAPLUS

CN 2-Propenoic acid, 3-(3-bromo-4,6-dihydroxy[1,1'-bipheny1]-2-y1)-, methy1

ester (CA INDEX NAME)

RN 860152-48-3 CAPLUS

CN 3-Buten-2-one, 4-(3-bromo-4,6-dihydroxy[1,1'-bipheny1]-2-y1)- (CA INDEX NAME)

RN 860152-49-4 CAPLUS

CN [1,1'-Bipheny1]-2,4-diol, 5-bromo-6-methoxy- (CA INDEX NAME)

RN 860152-50-7 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 5-bromo-6-(2-hydroxyethyl)- (CA INDEX NAME)

RN 860152-51-8 CAPLUS

CN [1,1'-Bipheny1]-2,4,6-triol, 3-bromo- (CA INDEX NAME)

RN 860152-52-9 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 5-bromo-6-(2-methoxyethyl)- (CA INDEX NAME)

RN 860152-53-0 CAPLUS

CN 2-Propanone, 1-(3-bromo-4,6-dihydroxy[1,1'-biphenyl]-2-yl)- (CA INDEX NAME)

$$\begin{array}{c|c} \text{Ph} & \bigcirc & \bigcirc \\ \text{HO} & \longrightarrow & \bigcirc \\ \text{Br} & \bigcirc & \text{Me} \end{array}$$

RN 860152-54-1 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-3'-(3-methoxy-3-oxo-1-propen-1-yl)-, methyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{MeC-} \overset{\circ}{\mathbb{L}} \text{CH}_2 \\ \text{HO} \end{array} \qquad \begin{array}{c} \text{CH-} \overset{\circ}{\mathbb{L}} \text{CH-} \overset{\circ}{\mathbb{L}} \text{OMe} \end{array}$$

RN 860152-55-2 CAPLUS

CN [1,1'-Biphenyl]-3-propanoic acid, 2',4'-dihydroxy-6'-(2-methoxy-2oxoethyl)- (CA INDEX NAME)

RN 860152-56-3 CAPLUS

CN [1,1'-Biphenyl]-3-propanoic acid, 3'-bromo-4',6'-dihydroxy-2'-(2-methoxy-2oxoethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} \longrightarrow \text{CH}_2 \\ \text{Br} \longrightarrow \text{CH}_2 \longrightarrow \text{CH}_2 \longrightarrow \text{CH}_2 \longrightarrow \text{CH}_2 \longrightarrow \text{CO}_2 \\ \text{Ho} \longrightarrow \text{CH}_2 \longrightarrow \text{CH}_2 \longrightarrow \text{CH}_2 \longrightarrow \text{CO}_2 \\ \text{Ho} \longrightarrow \text{CH}_2 \longrightarrow \text{CH}_$$

RN 860152-57-4 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 3-acetyl-4,6-dihydroxy-, methyl ester (CA INDEX NAME)

RN 860152-58-5 CAPLUS

$$\begin{array}{c} \text{Ph} & \text{CH}_2 - \text{OMe} \\ \text{CH}_2 - \text{Ph} \end{array}$$

RN 860152-59-6 CAPLUS

CN [1,1'-Bipheny1]-2,4-dio1, 5-bromo-6-[(2-methoxyethoxy)methy1]- (CA INDEX NAME)

RN 860152-60-9 CAPLUS

CN [1,1'-Bipheny]-2,4-dio1, 5-bromo-6-[[2-(2-methoxyethoxy)ethoxy]methy1](CA INDEX NAME)

RN 860152-61-0 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 4'-acetyl-4,6-dihydroxy-, methyl ester (CA INDEX NAME)

RN 860152-62-1 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-3'-(trifluoromethoxy)-, methyl ester (CA INDEX NAME)

RN 860152-63-2 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-4'-(trifluoromethoxy)-,
methyl ester (CA INDEX NAME)

RN 860152-64-3 CAPLUS

RN 860152-65-4 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-3'-nitro-, methyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{MeO-} \overset{\circ}{\text{C-}} \text{CH}_2 \\ \text{HO-} \overset{\circ}{\text{OH}} \end{array}$$

RN 860152-66-5 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 3'-cyano-4,6-dihydroxy-, methyl ester (CA INDEX NAME)

RN 860152-67-6 CAPLUS

CN [1,1':4',1''-Terphenyl]-2-acetic acid, 4,6-dihydroxy-, methyl ester (9CI)
(CA INDEX NAME)

- RN 860152-68-7 CAPLUS
- CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-4'-phenoxy-, methyl ester (CA INDEX NAME)

- RN 860152-69-8 CAPLUS
- CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-3'-methoxy-, methyl ester (CA INDEX NAME)

- RN 860152-70-1 CAPLUS
- CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-4'-methoxy-, methyl ester (CA INDEX NAME)

RN 860152-71-2 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 5-ethyl-6-(2-methoxyethyl)- (CA INDEX NAME)

RN 860152-72-3 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 5-ethyl-6-(2-hydroxyethyl)- (CA INDEX NAME)

RN 860152-73-4 CAPLUS

CN [1,1'-Biphenyl]-2,4-dio1, 5-bromo-6-[[(tetrahydro-2furanyl)methoxy]methyl]- (CA INDEX NAME)

RN 860152-74-5 CAPLUS

CN [1,1'-Bipheny1]-2,4-dio1, 5-bromo-6-[2-(2-methoxyethoxy)ethy1]- (CA INDEX NAME)

RN 860152-75-6 CAPLUS

CN [1,1'-Biphenyl]-2-propanoic acid, 3-bromo-4,6-dihydroxy-, methyl ester (CA INDEX NAME)

RN 860152-76-7 CAPLUS

CN Ethanone, 2-(3-bromo-4,6-dihydroxy[1,1'-biphenyl]-2-yl)-1-[4-(2-methoxyphenyl)-1-piperazinyl]- (CA INDEX NAME)

RN 860152-77-8 CAPLUS

CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N-methyl-N-[2-(2pyridinyl)ethyl]- (CA INDEX NAME)

RN 860152-78-9 CAPLUS

CN 3-Pyridinecarbonitrile, 2-[4-[2-(3-bromo-4,6-dihydroxy[1,1'-biphenyl]-2yl)acetyl]-1-piperazinyl]- (CA INDEX NAME)

RN 860152-79-0 CAPLUS

CN Ethanone, 2-(3-bromo-4,6-dihydroxy[1,1'-biphenyl]-2-yl)-1-[4-(2furanylcarbonyl)-1-piperazinyl]- (CA INDEX NAME)

RN 860152-80-3 CAPLUS

CN Ethanone, 1-[4,6-dihydroxy-2-(2-methoxyethyl)[1,1'-biphenyl]-3-yl]- (CA INDEX NAME)

RN 860152-81-4 CAPLUS

CN 1-Propanone, 1-[4,6-dihydroxy-2-(2-methoxyethyl)[1,1'-biphenyl]-3-yl]-2-methyl- (CA INDEX NAME)

RN 860152-82-5 CAPLUS

CN 1-Propanone, 1-[4,6-dihydroxy-2-(2-methoxyethy1)[1,1'-bipheny1]-3-y1](CA INDEX NAME)

RN 860152-83-6 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 6-(2-methoxyethyl)-5-propyl- (CA INDEX NAME)

RN 860152-84-7 CAPLUS

CN [1,1'-Biphenyl]-2,4-dio1, 6-(2-methoxyethyl)-5-(2-methylpropyl)- (CA INDEX NAME)

RN 860152-85-8 CAPLUS

CN [1,1'-Bipheny1]-2,4-diol, 5-bromo-6-(3-methoxypropy1)- (CA INDEX NAME)

RN 860152-87-0 CAPLUS

CN [1,1'-Biphenyl]-2,4-dio1, 5-bromo-6-[2-(dimethylamino)ethyl]- (CA INDEX NAME)

- RN 860152-88-1 CAPLUS
- CN [1,1'-Bipheny1]-2,4-diol, 5-bromo-6-[2-[(2-methoxyethyl)amino]ethyl]- (CA INDEX NAME)

- RN 860152-89-2 CAPLUS
- CN [1,1'-Bipheny1]-2,4-dio1, 5-bromo-6-[(methylamino)methyl]- (CA INDEX NAME)

- RN 860152-90-5 CAPLUS
- CN [1,1'-Biphenyl]-2,4-diol, 5-bromo-6-[(dimethylamino)methyl]- (CA INDEX NAME)

- RN 860152-91-6 CAPLUS

- RN 860152-92-7 CAPLUS
- CN [1,1'-Biphenyl]-2,4-diol, 5-bromo-6-(3-hydroxypropyl)- (CA INDEX NAME)

- RN 860152-93-8 CAPLUS

- RN 860152-94-9 CAPLUS
- CN [1,1'-Biphenyl]-3-carboxylic acid,
 3'-bromo-4',6'-dihydroxy-2'-(2-methoxyethyl)- (CA INDEX NAME)

- RN 860152-95-0 CAPLUS
- CN 2-Propanone, 1-(3-bromo-4,6-dihydroxy-3'-methoxy[1,1'-bipheny1]-2-y1)-, oxime (CA INDEX NAME)

- RN 860152-96-1 CAPLUS
- CN [1,1'-Bipheny1]-2,4-diol, 5-bromo-3'-methoxy-6-[2-[(tetrahydro-2H-pyran-2-

yl)methoxy]ethyl]- (CA INDEX NAME)

RN 860152-98-3 CAPLUS

CN [1,1'-Bipheny1]-2,4-dio1, 5-bromo-6-[2-(2-hydroxyethoxy)ethy1]- (CA INDEX NAME)

RN 860152-99-4 CAPLUS

CN [1,1'-Biphenyl]-2,4-dio1, 5-bromo-6-[2-(methoxymethoxy)ethyl]- (CA INDEX NAME)

RN 860153-00-0 CAPLUS

CN [1,1'-Bipheny1]-2,4-diol, 5-bromo-6-(1,3-dioxolan-2-y1)- (CA INDEX NAME)

RN 860153-01-1 CAPLUS

CN [1,1'-Bipheny1]-2,4-dio1, 5-ethyl-6-[2-(2-methoxyethoxy)ethyl]- (CA INDEX NAME)

RN 860153-02-2 CAPLUS

CN 2-Butanone, 4-(3-bromo-4,6-dihydroxy[1,1'-bipheny1]-2-y1)- (CA INDEX NAME)

RN 860153-03-3 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 5-bromo-6-(3-hydroxybutyl)- (CA INDEX NAME)

RN 860153-04-4 CAPLUS

CN Ethanone, 1-[4,6-dihydroxy-3'-methoxy-2-(2-methoxyethy1)[1,1'-bipheny1]-3y1]- (CA INDEX NAME)

RN 860153-05-5 CAPLUS

CN [1,1'-Bipheny1]-3-carboxamide, 3'-bromo-4',6'-dihydroxy-2'-(2methoxyethy1)- (CA INDEX NAME)

RN 860153-06-6 CAPLUS

CN [1,1'-Bipheny1]-2,4-dio1, 5-ethy1-3'-methoxy-6-(2-methoxyethy1)- (CA INDEX NAME)

RN 860153-07-7 CAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 3'-acetyl-4',6'-dihydroxy-2'-(2-methoxyethyl)-, methyl ester (CA INDEX NAME)

RN 860153-08-8 CAPLUS

RN 860153-09-9 CAPLUS

CN Ethanone, 1-[3'-ethoxy-4,6-dihydroxy-2-(2-methoxyethyl)[1,1'-biphenyl]-3-yl]- (CA INDEX NAME)

RN 860153-10-2 CAPLUS

CN Ethanone, 1-[4,6-dihydroxy-2-(2-methoxyethyl)-3'-methyl[1,1'-biphenyl]-3yl]- (CA INDEX NAME)

RN 860153-11-3 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 5-ethyl-6-(3-hydroxypropyl)- (CA INDEX NAME)

RN 860153-12-4 CAPLUS

CN Ethanone, 1-[4,6-dihydroxy-2-(3-hydroxypropy1)[1,1'-bipheny1]-3-y1]- (CA INDEX NAME)

RN 860153-13-5 CAPLUS

CN Ethanone, 1-[4,6-dihydroxy-2-(2-methoxyethyl)[1,1'-biphenyl]-3-yl]-2,2,2trifluoro- (CA INDEX NAME)

RN 860153-15-7 CAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 4,6-dihydroxy-2-(2-methoxyethyl)- (CA INDEX NAME)

RN 860153-16-8 CAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 4,6-dihydroxy-2-(2-methoxyethyl)-,
 methyl ester (CA INDEX NAME)

RN 860153-17-9 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 5-methoxy-6-(2-methoxyethyl)- (CA INDEX NAME)

RN 860153-18-0 CAPLUS

CN [1,1'-Biphenyl]-2,4-dio1, 5-ethyl-6-(2-methoxyethyl)-3'-methyl- (CA INDEX NAME)

RN 860153-19-1 CAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 3'-ethyl-4',6'-dihydroxy-2'-(2-methoxyethyl)-, methyl ester (CA INDEX NAME)

RN 860153-20-4 CAPLUS

CN [1,1':3',1''-Terphenyl]-2,4-diol, 5-ethyl-6-(2-methoxyethyl)- (9CI) (CA INDEX NAME)

RN 860153-21-5 CAPLUS

CN [1,1'-Bipheny1]-2,4-dio1, 3'-ethoxy-5-ethyl-6-(2-methoxyethyl)- (CA INDEX NAME)

RN 860153-22-6 CAPLUS

RN 860153-23-7 CAPLUS

CN Ethanone, 1-[4,6-dihydroxy-2-(2-methoxyethyl)-3'-(phenylmethoxy)[1,1'-biphenyl]-3-yl]- (CA INDEX NAME)

RN 860153-24-8 CAPLUS

CN Ethanone, 1-[4,6-dihydroxy-2-[2-(2-methoxyethoxy)ethyl][1,1'-biphenyl]-3yl]- (CA INDEX NAME)

RN 860153-25-9 CAPLUS

CN Ethanone, 1-[4,6-dihydroxy-3'-methoxy-2-[2-(2-methoxyethoxy)ethy1][1,1'-bipheny1]-3-y1]- (CA INDEX NAME)

RN 860153-26-0 CAPLUS

RN 860153-27-1 CAPLUS

CN Ethanone, 1-[4,6-dihydroxy-2-[2-(2-methoxyethoxy)ethy1]-3'-methy1[1,1'-bipheny1]-3-y1]- (CA INDEX NAME)

RN 860153-28-2 CAPLUS

CN Methanesulfonic acid, 1,1,1-trifluoro-,
 2-hydroxy-6-[2-(2-methoxyethoxy)ethyl][1,1'-biphenyl]-4-yl ester (CA INDEX NAME)

$$F_3C - \bigcup_{H} O - CH_2 - CH_2 - CH_2 - CH_2 - CH_2 - OMe$$

RN 860153-29-3 CAPLUS

CN [1,1'-Biphenyl]-2-acetamide, 3-acetyl-4,6-dihydroxy-3'-methoxy-N-(2methoxyethyl)-N-methyl- (CA INDEX NAME)

RN 860153-30-6 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 3-ethyl-4,6-dihydroxy-3'-methoxy-, methyl
ester (CA INDEX NAME)

RN 860153-31-7 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 5-ethyl-6-(2-hydroxyethyl)-3'-methoxy- (CA INDEX NAME)

RN 860153-32-8 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 5-ethyl-6-[2-(2-propen-1-yloxy)ethyl]- (CA INDEX NAME)

RN 860153-33-9 CAPLUS

RN 860153-35-1 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 6-[2-(2,3-dihydroxypropoxy)ethyl]-5-ethyl- (CA INDEX NAME)

RN 860153-36-2 CAPLUS

CN [1,1'-Bipheny1]-2,4-dio1, 6-[3-(2,3-dihydroxypropoxy)propy1]-5-ethyl- (CA INDEX NAME)

$$\begin{array}{c} \text{Ph} \\ \text{HO} \\ \end{array} \begin{array}{c} \text{OH} \\ \text{CH}_2 \text{) }_3 \text{----} \text{CH}_2 \text{---} \text{CH}_2 \text{---} \text{OH} \\ \\ \text{Et} \end{array}$$

RN 860153-37-3 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 5-ethyl-6-[2-(2-methoxyethoxy)ethyl]-3'-methyl-(CA INDEX NAME)

RN 860153-38-4 CAPLUS

CN [1,1'-Biphenyl]-2-acetamide, 3-ethyl-4,6-dihydroxy-3'-methoxy-N-(2methoxyethyl)-N-methyl- (CA INDEX NAME)

RN 860153-39-5 CAPLUS

CN [1,1'-Bipheny1]-2,4-dio1, 6-(2-methoxyethy1)-5-(1-methylethy1)- (CA INDEX NAME)

HO
$$CH_2$$
— CH_2 — OMe

RN 860153-40-8 CAPLUS

CN Sulfamic acid, 2-hydroxy-6-[2-(2-methoxyethoxy)ethyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\mathsf{H}_2 \mathbb{N} = \bigcup_{h=0}^{2} \mathsf{CH}_2 - \mathsf{CH}_2$$

RN 860153-41-9 CAPLUS

CN 2-Butanone, 4-[3'-ethyl-4',6'-dihydroxy-2'-[2-(2-methoxyethoxy)ethyl][1,1'-biphenyl]-3-yl]- (CA INDEX NAME)

$$\begin{array}{c} \text{OH} \\ \text{CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-OMe} \\ \text{CH}_2\text{-CH}_2\text{-CH}_2\text{-OMe} \\ \end{array}$$

RN 860153-42-0 CAPLUS

CN [1,1'-Biphenyl]-2,4-dio1, 5-ethyl-3'-(3-hydroxybutyl)-6-[2-(2methoxyethoxy)ethyl]- (CA INDEX NAME)

$$\begin{array}{c} \text{OH} & \text{OH} \\ \text{CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-Me} \\ \\ \text{HO} & \text{CH}_2\text{-CH}_2\text{-CH}_2\text{-OMe} \end{array}$$

RN 860153-43-1 CAPLUS

CN Acetamide, 2-[2-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)ethoxy]- (CA INDEX NAME)

RN 860153-44-2 CAPLUS

CN Acetamide, 2-[2-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)ethoxy]-N-methyl- (CA INDEX NAME)

RN 860153-45-3 CAPLUS

CN Acetamide, 2-[2-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)ethoxy]-N,N-dimethyl- (CA INDEX NAME)

$$\begin{array}{c} \text{Ph} \\ \text{CH}_2-\text{CH}_2-\text{O-} \text{CH}_2 \\ \end{array} \\ \begin{array}{c} \text{C} \\ \text{NMe}_2 \\ \end{array}$$

RN 860153-46-4 CAPLUS

CN Acetamide, 2-[3-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)propoxy]- (CA INDEX NAME)

$$\begin{array}{c} \text{Ph} \\ \text{HO} \\ \end{array} \begin{array}{c} \text{Ph} \\ \text{Et} \end{array} \begin{array}{c} \text{O} \\ \text{CH}_2 \text{) } 3 - \text{O} - \text{CH}_2 - \overset{\text{O}}{\text{CH}}_2 \text{NH}_2 \end{array}$$

RN 860153-47-5 CAPLUS

CN Acetamide, 2-[3-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)propoxy]-N-

methyl- (CA INDEX NAME)

RN 860153-48-6 CAPLUS

CN Acetamide, 2-[3-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)propoxy]-N,N-dimethyl- (CA INDEX NAME)

HO
$$(CH_2)_3 - O - CH_2 - O$$
 NMe_2

RN 860153-49-7 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 5-ethyl-6-[2-(2-hydroxyethoxy)ethyl]- (CA INDEX NAME)

RN 860153-50-0 CAPLUS

RN 860153-51-1 CAPLUS

CN [1,1'-Bipheny1]-2,4-dio1, 5-ethyl-6-[3-[2-hydroxy-1-

(hydroxymethyl)ethoxy]propyl]- (CA INDEX NAME)

RN 860153-52-2 CAPLUS

CN 2-Pyrrolidinone, 1-[3-[3-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)propoxy]propyl]- (CA INDEX NAME)

RN 860153-53-3 CAPLUS

CN Ethanone, 1-[3',4,6-trihydroxy-2-[2-(2-methoxyethoxy)ethyl][1,1'-biphenyl]-3-yl]- (CA INDEX NAME)

RN 860153-54-4 CAPLUS

CN [1,1'-Biphenyl]-2,3',4-triol, 5-ethyl-6-[2-(2-methoxyethoxy)ethyl]- (CA INDEX NAME)

- RN 860153-55-5 CAPLUS
- CN Acetamide, 2-[3-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)propoxy]-N-(2-hydroxyethyl)- (CA INDEX NAME)

- RN 860153-56-6 CAPLUS
- CN Acetamide, 2-[3-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)propoxy]-N-(2-methoxyethyl)- (CA INDEX NAME)

$$Ph$$
 $(CH_2)_3 - O - CH_2 - U - NH - CH_2 - CH_2 - OMe$

- RN 860153-57-7 CAPLUS

Relative stereochemistry.

- RN 860153-58-8 CAPLUS
- CN 1,2,4-Hexanetriol, 6-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)-, (2R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.

RN 860153-59-9 CAPLUS

CN [1,1'-Biphenyl]-2,3',4-triol, 5-ethyl-6-(2-methoxyethyl)- (CA INDEX NAME)

RN 860153-60-2 CAPLUS

CN [1,1'-Biphenyl]-2,3',4-triol, 5-ethyl-6-(2-hydroxyethyl)- (CA INDEX NAME)

RN 860153-61-3 CAPLUS

CN [1,1'-Biphenyl]-2,3',4-triol, 6-[2-(2,3-dihydroxypropoxy)ethyl]-5-ethyl-(CA INDEX NAME)

RN 860153-62-4 CAPLUS

CN [1,1'-Biphenyl]-2,3',4-trio1, 5-ethyl-6-[2-(2-hydroxyethoxy)ethyl]- (CA INDEX NAME)

RN 860153-63-5 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 5-ethyl-6-[2-(3-hydroxypropoxy)ethyl]- (CA INDEX NAME)

RN 860153-64-6 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 5-ethyl-6-[2-(3-methoxypropoxy)ethyl]- (CA INDEX NAME)

RN 860153-65-7 CAPLUS

CN erythro-Pentitol, 3,5-dideoxy-5-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 860153-66-8 CAPLUS

CN threo-Pentitol, 1,3-dideoxy-1-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)(CA INDEX NAME)

Relative stereochemistry.

RN 860153-67-9 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 5-ethyl-6-[2-[2-hydroxy-3-(2-hydroxyethoxy)propoxy]ethyl]- (CA INDEX NAME)

RN 860153-68-0 CAPLUS

RN 860153-69-1 CAPLUS

$$\begin{array}{c} \text{Et} & \text{OH} & \text{OH} & \text{OH} \\ \text{HO} & \text{CH}_2\text{--}\text{CH}_2\text{--}\text{CH}_2\text{--}\text{CH}_2\text{--}\text{OH} \\ \end{array}$$

RN 860153-70-4 CAPLUS

CN [1,1'-Bipheny1]-2,4-dio1, 6-(2,3-dihydroxypropy1)-5-ethyl- (CA INDEX

NAME)

$$\operatorname{HO} \longrightarrow \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname{OH}$$

RN 860153-71-5 CAPLUS

CN α-D-Glucopyranoside, 2-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)ethyl (CA INDEX NAME)

Absolute stereochemistry.

RN 860153-72-6 CAPLUS

CN Propanedioic acid, 2-[3-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)-1hydroxypropyl]-, 1,3-diethyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{ of } \\ \text{OH} \\ \text{OH} \\ \text{Ph} \\ \text{OH} \end{array}$$

RN 860153-73-7 CAPLUS

CN [1,1'-Biphenyl]-2,4-dio1, 6-[3,5-dihydroxy-4-(hydroxymethyl)pentyl]-5ethyl- (CA INDEX NAME)

RN 860153-74-8 CAPLUS

CN [1,1'-Biphenyl]-2-propanamide, 3-acetyl-4,6-dihydroxy-N,N-bis(2hydroxyethyl)- (CA INDEX NAME)

RN 860153-75-9 CAPLUS

CN [1,1'-Biphenyl]-2-propanamide, 3-ethyl-4,6-dihydroxy-N,N-bis(2-hydroxyethyl)- (CA INDEX NAME)

RN 860153-76-0 CAPLUS

RN 860153-77-1 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 6-[2-(2,3-dihydroxypropoxy)ethyl]-5-ethyl-3'methoxy- (CA INDEX NAME)

- RN 860153-78-2 CAPLUS
- CN [1,1'-Biphenyl]-2,4-dio1, 6-[2-(2,3-dihydroxypropoxy)ethyl]-5-ethyl-3'-(2pyridinylmethoxy)- (CA INDEX NAME)

- RN 860153-79-3 CAPLUS
- CN [1,1'-Biphenyl]-2,4-diol, 6-[2-(2,3-dihydroxypropoxy)ethyl]-5-ethyl-3'-(3pyridinylmethoxy)- (CA INDEX NAME)

$$\begin{array}{c} \text{HO} & \text{OH} \\ \text{N} & \text{CH}_{2}\text{--}\text{O} \\ \text{CH}_{2}\text{--}\text{CH}_{2}\text{--}\text{O} \\ \text{CH}_{2}\text{--}\text{CH}_{2}\text{--}\text{OH} \\ \end{array}$$

- RN 860153-80-6 CAPLUS
- CN [1,1'-Bipheny1]-2,4-dio1, 6-[2-(2,3-dihydroxypropoxy)ethy1]-5-ethyl-3'-(4-pyridinylmethoxy)- (CA INDEX NAME)

- RN 860153-81-7 CAPLUS
- CN [1,1'-Biphenyl]-2,4-dio1, 6-[2-(2,3-dihydroxypropoxy)ethyl]-5-ethyl-3'-[(2methyl-4-thiazolyl)methoxy]- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} & \text{OH} \\ \text{S} & \text{CH}_2-\text{OH}_2-\text{O-CH}_2-\text{CH-CH}_2-\text{OH} \\ \text{L}_{1...} & \text{L}_{1...} \end{array}$$

- RN 860153-82-8 CAPLUS
- CN [1,1'-Biphenyl]-2,4-dio1, 6-[2-(2,3-dihydroxypropoxy)ethyl]-5-ethyl-3'-(2hydroxyethoxy)- (CA INDEX NAME)

- RN 860153-83-9 CAPLUS
- CN [1,1'-Biphenyl]-2,4-diol, 6-[2-(2,3-dihydroxypropoxy)ethyl]-5-ethyl-3'-[2-(4-morpholinyl)ethoxy]- (CA INDEX NAME)

- RN 860153-84-0 CAPLUS
- CN 2-Pyrrolidinone, 1-[2-[[2'-[2-(2,3-dihydroxypropoxy)ethyl]-3'-ethyl-4',6'dihydroxy[1,1'-biphenyl]-3-yl]oxy]ethyl]- (CA INDEX NAME)

CN [1,1'-Biphenyl]-2,4-diol, 3'-amino-6-[2-(2,3-dihydroxypropoxy)ethyl]-5ethyl- (CA INDEX NAME)

- RN 860153-86-2 CAPLUS

- RN 860153-87-3 CAPLUS

- RN 860153-88-4 CAPLUS
- CN 4-Oxazolecarboxylic acid, 5-[(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2yl)methyl]-, methyl ester (CA INDEX NAME)

- RN 860153-89-5 CAPLUS
- CN D-arabino-Hexopyranoside, 2-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)ethyl 2-deoxy- (CA INDEX NAME)

- RN 860153-90-8 CAPLUS
- CN Methanesulfonamide, N-[2'-[2-(2,3-dihydroxypropoxy)ethyl]-3'-ethyl-4',6'dihydroxy[1,1'-biphenyl]-3-yl]- (CA INDEX NAME)

$$\begin{array}{c} \text{OH} \\ \text{HO} \\ \text{Et} \end{array} \begin{array}{c} \text{OH} \\ \text{CH}_2-\text{CH}_2-\text{O} \\ \text{CH}_2-\text{CH}_2-\text{CH} \end{array} \begin{array}{c} \text{OH} \\ \text{CH}_2-\text{OH} \\ \text{CH}_2-\text{OH} \end{array}$$

- RN 860153-91-9 CAPLUS
- CN Benzenesulfonamide, N-[2'-[2-(2,3-dihydroxypropoxy)ethyl]-3'-ethyl-4',6'-dihydroxy[1,1'-biphenyl]-3-yl]-4-methyl- (CA INDEX NAME)

- RN 860153-92-0 CAPLUS
- CN Acetamide, N-[2'-[2-(2,3-dihydroxypropoxy)ethyl]-3'-ethyl-4',6'-dihydroxy[1,1'-biphenyl]-3-yl]- (CA INDEX NAME)

$$\begin{array}{c} \circ H \\ \text{HO-CH}_2- \overset{\circ}{\text{CH}}_2- \circ - \text{CH}_2- \text{CH}_2 \\ \text{Et} \\ \text{HO} \end{array}$$

RN 860153-93-1 CAPLUS

CN Benzamide, N-[2'-[2-(2,3-dihydroxypropoxy)ethyl]-3'-ethyl-4',6'dihydroxy[1,1'-biphenyl]-3-yl]- (CA INDEX NAME)

RN 860153-94-2 CAPLUS

CN Urea, N-[2'-[2-(2,3-dihydroxypropoxy)ethyl]-3'-ethyl-4',6'-dihydroxy[1,1'-biphenyl]-3-yl]-N'-ethyl- (CA INDEX NAME)

RN 860153-95-3 CAPLUS

CN Propanamide, N-[2'-[2-(2,3-dihydroxypropoxy)ethyl]-3'-ethyl-4',6'-dihydroxy[1,1'-biphenyl]-3-yl]-3-hydroxy-2-(hydroxymethyl)-2-methyl- (CA INDEX NAME)

RN 860153-96-4 CAPLUS

 $\label{eq:cn_loss} \begin{tabular}{ll} CN & [1,1'-Biphenyl]-2,4-diol, & 5-ethyl-6-[[4-(hydroxymethyl)-5-oxazolyl]methyl]-1 & (hydroxymethyl)-5-oxazolyl]methyl]-1 & (hydroxymethyl)-1 &$

(CA INDEX NAME)

RN 860153-97-5 CAPLUS

CN 4-Oxazolecarboxylic acid, 5-[2-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2yl)ethyl]-, methyl ester (CA INDEX NAME)

RN 860153-98-6 CAPLUS

CN [1,1'-Biphenyl]-2,4-dio1, 5-ethyl-6-[2-[4-(hydroxymethyl)-5oxazolyl]ethyl]- (CA INDEX NAME)

RN 860153-99-7 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 5-ethyl-6-[[4-(hydroxymethyl)-1,3-dioxolan-2yl]methyl]- (CA INDEX NAME)

RN 860154-00-3 CAPLUS

CN [1,1'-Biphenyl]-2-propanamide, 3-ethyl-4,6-dihydroxy- (CA INDEX NAME)

RN 860154-01-4 CAPLUS

CN Propanedioic acid, 2-[2-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)ethyl], 1,3-dimethyl ester (CA INDEX NAME)

RN 860154-03-6 CAPLUS

CN [1,1'-Bipheny1]-2,4-dio1, 5-ethyl-6-[4-hydroxy-3-(hydroxymethyl)butyl](CA INDEX NAME)

RN 860154-04-7 CAPLUS

CN D-lyxo-Hexopyranoside, 2-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)ethyl
2-deoxy- (CA INDEX NAME)

Absolute stereochemistry.

RN 860154-05-8 CAPLUS

CN [1,1'-Biphenyl]-2,4-dio1, 5-ethyl-6-[5-hydroxy-4-(hydroxymethyl)pentyl](CA INDEX NAME)

RN 860154-06-9 CAPLUS

CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2yl)methyl]-, (4R,5R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 860154-07-0 CAPLUS

CN [1,1'-Bipheny1]-2,3',4-triol, 5-ethyl-6-[2-(2-oxiranylmethoxy)ethyl]- (CA INDEX NAME)

RN 860154-08-1 CAPLUS

CN [1,1'-Biphenyl]-2-propanamide, 3-ethyl-4,6-dihydroxy-N-(2-hydroxyethyl)-(CA INDEX NAME)

RN 860154-09-2 CAPLUS

CN [1,1'-Biphenyl]-2-propanamide, N-[2-(acetylamino)ethyl]-3-ethyl-4,6-dihydroxy- (CA INDEX NAME)

$$\begin{array}{c} \text{ bt } & \text{ ch}_2\text{-ch}_2\text{-ch}_2\text{-nh-ch}_2\text{-ch}_2\text{-nhac} \\ & \text{ ph } \end{array}$$

RN 860154-10-5 CAPLUS

CN 4-Oxazolecarboxamide, 5-[2-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2yl)ethyl]- (CA INDEX NAME)

RN 860154-11-6 CAPLUS

CN 4-Oxazolecarboxamide, 5-[2-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2yl)ethyl]-N-(2-hydroxyethyl)- (CA INDEX NAME)

- RN 860154-12-7 CAPLUS
- CN 4-Oxazolecarboxamide, 5-[2-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2yl)ethyl|-N,N-bis(2-hydroxyethyl)- (CA INDEX NAME)

- RN 860154-13-8 CAPLUS
- CN 4-Oxazolecarboxamide, 5-[2-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)ethyl]-N-[2-hydroxy-1-(hydroxymethyl)ethyl]- (CA INDEX NAME)

- RN 860154-14-9 CAPLUS
- CN 4-Oxazolecarboxamide, N-(2,3-dihydroxypropyl)-5-[2-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)ethyl]- (CA INDEX NAME)

$$\begin{array}{c} O\\ O\\ C\\ H_2\\ C\\ H_2\\ C\\ H_2\\ D\\ H_2\\ D$$

RN 860154-15-0 CAPLUS

CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-4,6-dihydroxy-3'-methyl[1,1'-biphenyl]-2-yl)methyl]-, (4R,5R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 860154-16-1 CAPLUS

CN 1,3-Dioxolane-4,5-dimethanol, 2-[(4,6-dihydroxy[1,1'-biphenyl]-2yl)methyl]-, (4R,5R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 860154-18-3 CAPLUS

CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-bromo-4,6-dihydroxy[1,1'-biphenyl]-2yl)methyl]-, (4R,5R)- (CA INDEX NAME)

RN 860154-19-4 CAPLUS

CN 1,3-Dioxolane-4,5-dimethano1, 2-[(3-ethyl-4,6-dihydroxy-3'-methoxy[1,1'-biphenyl]-2-y1)methyl]-, (4S,5S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 860154-20-7 CAPLUS

CN Ethanone, 1-[2-[(4R,5R)-4,5-bis(hydroxymethy1)-1,3-dioxolan-2-y1]methy1]-4,6-dihydroxy[1,1'-bipheny1]-3-y1]- (CA INDEX NAME)

Absolute stereochemistry.

RN 860154-66-1 CAPLUS

CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-chloro-4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]-, (4R,5R)- (CA INDEX NAME)

RN 860154-67-2 CAPLUS

CN [1,1'-Biphenyl]-2,3',4-triol, 6-[[(4S,5S)-4,5-bis(hydroxymethyl)-1,3dioxolan-2-yl]methyl]-5-ethyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 860154-68-3 CAPLUS

CN 1,3-Dioxolane-4,5-dimethano1, 2-[(3-ethyl-3'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]-, (4S,5S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 860154-69-4 CAPLUS

CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-4,6-dihydroxy-3',5'-dimethyl[1,1'-biphenyl]-2-yl)methyl]-, (4S,5S)- (CA INDEX NAME)

- RN 860154-70-7 CAPLUS
- CN Acetamide, N-[2'-[[(4\$,5\$)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-3'-ethyl-4',6'-dihydroxy[1,1'-biphenyl]-3-yl]- (CA INDEX NAME)

Absolute stereochemistry.

- RN 860154-71-8 CAPLUS
- CN [1,1'-Biphenyl]-3-carboxamide, 2'-[[(4S,5S)-4,5-bis(hydroxymethyl)-1,3dioxolan-2-yl]methyl]-3'-ethyl-4',6'-dihydroxy- (CA INDEX NAME)

Absolute stereochemistry.

- RN 860154-72-9 CAPLUS
- CN [1,1'-Biphenyl]-3-carboxamide, 2'-[[(4\$,5\$)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-3'-ethyl-4',6'-dihydroxy-N-methyl- (CA INDEX NAME)

RN 860154-73-0 CAPLUS

CN [1,1'-Biphenyl]-3-carboxamide, 2'-[[(48,58)-4,5-bis(hydroxymethyl)-1,3dioxolan-2-yl]methyl]-3'-ethyl-4',6'-dihydroxy-N,N-dimethyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 860154-74-1 CAPLUS

CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-4'-fluoro-4,6-dihydroxy-3'methyl[1,1'-biphenyl]-2-yl)methyl]-, (48,5S)- (CA INDEX NAME)

Absolute stereochemistry.

IT 860154-78-52 860154-76-32 860154-77-48
860154-78-52 860154-76-67 860154-80-99
860154-78-59 860154-80-67 860154-80-99
860154-8-32 860154-80-18 860154-82-28
860154-8-32 860154-80-78 860154-86-59
860154-8-9-18 860154-87-8 860154-89-69
860154-90-18 860154-91-22 860154-92-39
860154-90-18 860154-91-22 860154-92-39
860154-96-78 860154-91-22 860154-92-39
860154-96-78 860154-91-22 860154-92-39
860153-90-67 860154-19-28 860174-21-67
860174-22-78 860293-33-68
860293-36-59 860293-39-68 860293-40-99
860293-41-09 860293-41-8 860293-40-99
860293-41-09 860293-45-48 860293-40-99
860293-41-69 860293-46-78 860293-45-59
861293-47-68 860293-46-78 860293-85-59
861293-47-68 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-46-78 860293-85-59
861293-47-86 860293-860293

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(benzene derivs. as Hsp90 family protein inhibitors and antitumor agents)

- RN 860154-75-2 CAPLUS
- CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3'-chloro-3-ethyl-4'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]-, (4R,5R)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 860154-76-3 CAPLUS
- CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-3',4'-difluoro-4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]-, (4R,5R)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 860154-77-4 CAPLUS
- CN [1,1'-Biphenyl]-3-carboxamide, 2'-[(4R,5R)-4,5-bis(hydroxymethyl)-1,3dioxolan-2-yl]methyl]-3'-ethyl-4',6'-dihydroxy-N-(2-methoxyethyl)- (CA INDEX NAME)

RN 860154-78-5 CAPLUS

CN [1,1'-Biphenyl]-3-carboxamide, 2'-[[(4R,5R)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-3'-ethyl-4',6'-dihydroxy-N-(2-hydroxyethyl)- (CA INDEX NAME)

Absolute stereochemistry.

RN 860154-79-6 CAPLUS

CN [1,1'-Biphenyl]-3-carboxamide, 2'-[[(4R,5R)-4,5-bis(hydroxymethyl)-1,3dioxolan-2-yl]methyl]-N-cyclopropyl-3'-ethyl-4',6'-dihydroxy- (CA INDEX NAME)

- RN 860154-80-9 CAPLUS
- CN [1,1'-Biphenyl]-3-carboxamide, 2'-[[(4R,5R)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-3'-ethyl-4',6'-dihydroxy-N-propyl- (CA INDEX NAME)

Absolute stereochemistry.

- RN 860154-81-0 CAPLUS
- CN [1,1'-Biphenyl]-2,3',4-triol, 6-[[(4R,5R)-4,5-bis(methoxymethyl)-1,3dioxolan-2-yl]methyl]-5-ethyl- (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c} \text{MeO} \\ \text{MeO} \\ \text{R} \end{array} \begin{array}{c} \text{OH} \\ \text{Et} \\ \text{OH} \end{array}$$

- RN 860154-82-1 CAPLUS
- CN [1,1'-Biphenyl]-2,4-dio1, 6-[[(4R,5R)-4,5-bis(methoxymethyl)-1,3-dioxolan-2-yl]methyl]-5-ethyl- (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} \\ \text{MeO} \\ \text{R} \\ \end{array} \begin{array}{c} \text{Ph} \\ \text{Ph} \\ \end{array}$$

- RN 860154-83-2 CAPLUS
- CN [1,1'-Biphenyl]-2,4-dio1, 5-ethyl-6-[2-(2-hydroxyethoxy)ethyl]-3',4'dimethoxy- (CA INDEX NAME)

RN 860154-84-3 CAPLUS

CN Ethanone, 1-[3',4,6-trihydroxy-2-[2-(2-hydroxyethoxy)ethy1][1,1'-bipheny1]3-y1]- (CA INDEX NAME)

RN 860154-85-4 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 3'-chloro-5-ethyl-4'-fluoro-6-[2-(2hydroxyethoxy)ethyl]- (CA INDEX NAME)

RN 860154-86-5 CAPLUS

CN 4-Oxazolecarboxylic acid, 2-[(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2yl)methyl]-4,5-dihydro-, methyl ester (CA INDEX NAME)

$$\text{MeO} = \bigcup_{i=1}^{N} \bigvee_{i=1}^{N} \bigcup_{i=1}^{N} \bigcup_{i=1}$$

RN 860154-87-6 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 5-ethyl-4'-fluoro-6-[2-(2-hydroxyethoxy)ethyl]-3'-methyl- (CA INDEX NAME)

- RN 860154-88-7 CAPLUS
- CN 1,3,4-Oxadiazol-2(3H)-one, 5-[(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2yl)methyl]- (CA INDEX NAME)

- RN 860154-89-8 CAPLUS
- CN [1,1'-Bipheny1]-2,4-dio1, 5-ethyl-6-[2-[(2S)-2-(hydroxymethyl)-1pyrrolidinyl]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.

- RN 860154-90-1 CAPLUS
- CN 1,3,4-Oxadiazol-2(3H)-one, 5-[(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2yl)methyl]-3-(2-methoxyethyl)- (CA INDEX NAME)

- RN 860154-91-2 CAPLUS
- CN 1,3,4-Oxadiazol-2(3H)-one, 5-[(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2yl)methyl]-3-(2-hydroxyethyl)- (CA INDEX NAME)

- RN 860154-92-3 CAPLUS

- RN 860154-93-4 CAPLUS
- CN [1,1'-Biphenyl]-2,4-dio1, 5-ethyl-6-[2-(3-hydroxy-1-pyrrolidinyl)ethyl](CA INDEX NAME)

- RN 860154-94-5 CAPLUS
- CN [1,1'-Biphenyl]-2-acetamide, 3-ethyl-4,6-dihydroxy-N-(2-hydroxyethyl)-N-(3methoxypropyl)- (CA INDEX NAME)

RN 860154-95-6 CAPLUS

CN 1,3,4-Oxadiazol-2(3H)-one, 5-[(3-ethyl-4,6-dihydroxy-3'-methoxy[1,1'-biphenyl]-2-y1)methyl]-3-(2-hydroxyethyl)- (CA INDEX NAME)

RN 860154-96-7 CAPLUS

CN 1,3,4-Oxadiazol-2(3H)-one, 5-[(3-ethyl-3',4,6-trihydroxy[1,1'-biphenyl]-2yl)methyl]-3-(2-methoxyethyl)- (CA INDEX NAME)

$$\text{MeO-CH2-CH2} \xrightarrow{\text{HO}} \xrightarrow{\text{CH2-CH2}} \xrightarrow{\text{OH}} \xrightarrow{\text{OH}}$$

RN 860154-97-8 CAPLUS

CN Carbonic acid, 5-ethyl-6-[2-(2-methoxyethoxy)ethyl][1,1'-biphenyl]-2,4diyl diethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{EtO} \\ \text{C} \\ \text{D} \\ \text{C} \\ \text{D} \\ \text{C} \\ \text{D} \\ \text{C} \\ \text{H}_{2} \\ \text{C} \\$$

- RN 860154-98-9 CAPLUS
- CN Carbamic acid, dimethyl-, 5-ethyl-6-[2-(2-methoxyethoxy)ethyl][1,1'-biphenyl]-2,4-diyl ester (9CI) (CA INDEX NAME)

- RN 860155-00-6 CAPLUS

- RN 860174-19-2 CAPLUS
- CN Ethanone, 1-(4-acetyl-1-piperazinyl)-2-(3-bromo-4,6-dihydroxy[1,1'-biphenyl]-2-yl)- (CA INDEX NAME)

- RN 860174-21-6 CAPLUS
- CN [1,1'-Biphenyl]-2,4-diol, 5-bromo-6-[2-(methylamino)ethyl]- (CA INDEX NAME)

RN 860174-22-7 CAPLUS

CN 4-Oxazolecarboxylic acid, 3-[2-(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)ethyl]-2,3-dihydro-2-oxo-, methyl ester (CA INDEX NAME)

RN 860293-36-3 CAPLUS

CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2yl)methyl]-, (4S,5S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 860293-37-4 CAPLUS

CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-4,6-dihydroxy-3'-methyl[1,1'-biphenyl]-2-yl)methyl]-, (49,58)- (CA INDEX NAME)

Absolute stereochemistry.

RN 860293-38-5 CAPLUS

CN 1,3-Dioxolane-4,5-dimethano1, 2-[(3-chloro-4,6-dihydroxy[1,1'-biphenyl]-2-v1)methyl]-, (4S.5S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 860293-39-6 CAPLUS

CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-4,6-dihydroxy-3'-methoxy[1,1'-biphenyl]-2-yl)methyl]-, (4R,5R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 860293-40-9 CAPLUS

CN Ethanone, 1-[2-[[(4S,5S)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]4,6-dihydroxy[1,1'-biphenyl]-3-yl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 860293-41-0 CAPLUS

CN [1,1'-Bipheny1]-3-carboxamide, 2'-[[(4R,5R)-4,5-bis(hydroxymethy1)-1,3-dioxolan-2-y1]methy1]-3'-ethy1-4',6'-dihydroxy-N,N-dimethy1- (CA INDEX

Absolute stereochemistry.

RN 860293-42-1 CAPLUS

CN [1,1'-Biphenyl]-3-carboxamide, 2'-[[(4R,5R)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-3'-ethyl-4',6'-dihydroxy-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 860293-43-2 CAPLUS

CN [1,1'-Biphenyl]-3-carboxamide, 2'-[[(4R,5R)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-3'-ethyl-4',6'-dihydroxy- (CA INDEX NAME)

Absolute stereochemistry.

RN 860293-44-3 CAPLUS

CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-3'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-2-y1)methyl]-, (4R,5R)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 860293-45-4 CAPLUS
- CN [1,1'-Biphenyl]-2,3',4-triol, 6-[[(4R,5R)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-5-ethyl- (CA INDEX NAME)

Absolute stereochemistry.

- RN 860293-46-5 CAPLUS
- CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-3',4'-difluoro-4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]-, (4S,5S)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 860293-47-6 CAPLUS
- CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3'-chloro-3-ethyl-4'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]-, (48,5S)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 860293-48-7 CAPLUS
- CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2yl)methyl]-, (4R,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.

- RN 860293-62-5 CAPLUS
- CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-4'-fluoro-4,6-dihydroxy-3'-methyl[1,1'-biphenyl]-2-yl)methyl]-, (4R,5R)- (CA INDEX NAME)

Absolute stereochemistry.

- IT 860156-38-3P 860156-39-4P 860156-40-7P
 - 860156-41-8P 860156-51-0P 860156-57-6P
 - 860156-63-4P 860156-96-3P 860157-27-3P
 - 860293-52-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(benzene derivs. as Hsp90 family protein inhibitors and antitumor agents)

- RN 860156-38-3 CAPLUS
- CN Carbonic acid, 5-ethyl-6-(2-methoxyethyl)-3'-methyl[1,1'-biphenyl]-2,4-diyl dimethyl ester (9CI) (CA INDEX NAME)

- RN 860156-39-4 CAPLUS
- CN [1,1"-Biphenyl]-3-carboxylic acid, 3'-ethyl-4',6'-bis[(methoxycarbonyl)oxy]-2'-(2-methoxyethyl)-, methyl ester (CA INDEX NAME)

- RN 860156-40-7 CAPLUS
- CN Carbonic acid, 5-ethyl-6-(2-methoxyethyl)[1,1':3',1''-terphenyl]-2,4-diyl dimethyl ester (9CI) (CA INDEX NAME)

- RN 860156-41-8 CAPLUS
- CN Carbonic acid, 3'-ethoxy-5-ethyl-6-(2-methoxyethyl)[1,1'-biphenyl]-2,4diyl dimethyl ester (9CI) (CA INDEX NAME)

- RN 860156-51-0 CAPLUS
- CN Carbonic acid, 5-ethyl-3'-methoxy-6-[2-(2-methoxyethoxy)ethyl][1,1'-biphenyl]-2,4-diyl dimethyl ester (9CI) (CA INDEX NAME)

- RN 860156-57-6 CAPLUS

- RN 860156-63-4 CAPLUS
- CN Carbonic acid, 5-ethyl-6-[2-(2-methoxyethoxy)ethyl]-3'-methyl[1,1'-biphenyl]-2,4-diyl dimethyl ester (9CI) (CA INDEX NAME)

- RN 860156-96-3 CAPLUS
- CN Carbonic acid, 5-ethyl-3'-hydroxy-6-(2-methoxyethyl)[1,1'-biphenyl]-2,4diyl dimethyl ester (9CI) (CA INDEX NAME)

RN 860157-27-3 CAPLUS

CN [1,1'-Biphenyl]-2-propanoic acid, 3-acetyl-4,6-dihydroxy- (CA INDEX NAME)

RN 860293-52-3 CAPLUS

CN 1,3-Dioxolane-4,5-dimethanol, 2-[(4,6-dihydroxy[1,1'-biphenyl]-2-v1)methyl]-, (48,58)- (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1991:196388 CAPLUS Full-text

DOCUMENT NUMBER: 114:196388 ORIGINAL REFERENCE NO.: 114:32930h,32931a

TITLE: Positive-working resist compositions

INVENTOR(S): Oie, Masayuki; Kaneko, Harumi; Mihira, Takayuki

PATENT ASSIGNEE(S): Nippon Zeon Co., Ltd., Japan SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF
DOCUMENT TYPE: Patent

LANGUAGE: Japanese FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

JP 02296247 A 19901206 JP 1989-118161 19890511

JP 02296247 A 19901206 JP 1989-118161 19890511 PRIORITY APPLN. INFO.: JP 1989-118161 19890511

AB The title compns. contain alkali-soluble phenol-containing resins and quinonediazidesulfonate esters of I (RI-4 = H, halo, alkyl, alkoxy; $5 \le m + n \le 6$). These resists are suitable for pattern formation with $\le 1-m$ resolution Thus, a composition containing 100 parts 6:4 m-cresol-p-cresol novolak and 20 parts II $\ge 95\%$ esterified with 1,2-naphthoqunonediazide-5-sulfonic acid was applied to a %1 wafer and prebaked to obtain a 1.17- μ m-thick resist layer. Patternwise exposure to g-line and development with aqueous Me4NOH gave a resist pattern with 0.45- μ m lines and spaces and 1.15 μ m thick. This pattern was used as a mask for dry etching in CF4 plasma.

IT 133404-50-9

RL: USES (Uses)

(pos.-working photoresist containing phenolic resins and)

RN 133404-50-9 CAPLUS

CN 1-Naphthalenesulfonic acid, 6-diazo-5,6-dihydro-5-oxo-, ester with 3-chloro[1,1'-biphenyl]-2,3',4,5',6-pentol (9CI) (CA INDEX NAME)

CM 1

CRN 199981-76-5 CMF C12 H9 C1 O5

CM 2

CRN 20546-03-6 CMF C10 H6 N2 O4 S

```
When nA is 1-5:
```

```
VAR G2=H/17/18/20/22/24/26/29/32/34
```

```
NODE ATTRIBUTES:
```

CONNECT IS E2 RC AT

CONNECT IS X4 RC AT 19 CONNECT IS X4 RC AT 25 CONNECT IS X4 RC AT 28 CONNECT IS X4 RC AT 31 CONNECT IS E1 RC AT 33 CONNECT IS X4 RC AT 35 CONNECT IS X4 RC AT 39 DEFAULT MLEVEL IS ATOM GGCAT IS LOC UNS AT 17 GGCAT IS LOC SAT AT 19 GGCAT IS LOC SAT AT 25 GGCAT IS LOC SAT AT 28 GGCAT IS LOC SAT AT 31 GGCAT IS UNS AT 35 GGCAT IS LOC SAT AT 39

GRAPH ATTRIBUTES: RSPEC 6 9

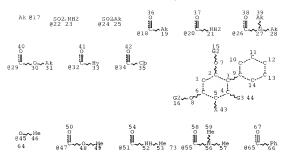
NUMBER OF NODES IS 42

STEREO ATTRIBUTES: NONE

DEFAULT ECLEVEL IS LIMITED

L3 869 SEA FILE=REGISTRY SSS FUL L1

1.7 STR



```
Page 2-A
VAR G2=H/17/18/20/22/24/26/29/32/34
VAR G3=OH/45/COOH/47/20/51/55/60/65/68/76/77
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 1
CONNECT IS X4 RC AT 19
CONNECT IS X4 RC AT 25
CONNECT IS X4 RC AT 28
CONNECT IS X4 RC AT 31
CONNECT IS E1 RC AT 33
CONNECT IS X4 RC AT 35
CONNECT IS X4 RC AT 39
CONNECT IS E2 RC AT 73
CONNECT IS E2 RC AT 74
CONNECT IS E3 RC AT 76
DEFAULT MLEVEL IS ATOM
GGCAT IS LOC UNS AT 17
GGCAT IS LOC SAT AT 19
GGCAT IS LOC SAT AT 25
GGCAT IS LOC SAT AT 28
GGCAT IS LOC SAT AT 31
GGCAT IS UNS AT 35
GGCAT IS LOC SAT AT 39
```

GRAPH ATTRIBUTES: RSPEC 6 9

DEFAULT ECLEVEL IS LIMITED

STEREO ATTRIBUTES: NONE

L9 15 SEA FILE=REGISTRY SUB=L3 SSS FUL L7

L10 2 SEA FILE=CAPLUS SPE=ON ABB=ON PLU=ON L9

L12 STR

60

CONNECT IS E2 RC AT 64

Page 2-A VAR G2=H/17/18/20/22/24/26/29/32/34 VAR G4=H/X/CN/NO2/45/46/48/49/NH2/52/55/COOH/57/61/63/64/66 NODE ATTRIBUTES: CONNECT IS E2 RC AT CONNECT IS X4 RC AT 19 CONNECT IS X4 RC AT 25 CONNECT IS X4 RC AT 28 CONNECT IS X4 RC AT 31 CONNECT IS E1 RC AT 33 CONNECT IS X4 RC AT 35 RC AT 39 CONNECT IS X4 CONNECT IS X4 RC AT 45 CONNECT IS X4 RC AT 47 CONNECT IS X4 RC AT 48 CONNECT IS X4 RC AT 50 CONNECT IS E1 RC AT 53 CONNECT IS E1 RC AT 54 CONNECT IS E1 RC AT 56 CONNECT IS X4 RC AT 59 CONNECT IS X4 RC AT 62 CONNECT IS X5 RC AT 63

```
CONNECT IS X4 RC AT 65
CONNECT IS E2 RC AT 66
CONNECT IS X4 RC AT 67
DEFAULT MLEVEL IS ATOM
GGCAT IS LOC UNS AT 17
GGCAT IS LOC SAT AT 19
GGCAT IS LOC SAT AT 25
GGCAT IS LOC SAT AT 28
GGCAT IS LOC SAT AT 31
GGCAT IS UNS AT 35
GGCAT IS LOC SAT AT 39
GGCAT IS LOC AT 45
GGCAT IS LOC SAT AT 47
GGCAT IS SAT AT 48
GGCAT IS LOC SAT AT 50
GGCAT IS LOC SAT AT 53
GGCAT IS LOC SAT AT 54
GGCAT IS LOC SAT AT 56
GGCAT IS LOC SAT AT 59
GGCAT IS UNS AT 62
GGCAT IS UNS AT 63
GGCAT IS SAT AT 64
GGCAT IS UNS AT 65
GGCAT IS SAT AT 66
DEFAULT ECLEVEL IS LIMITED
```

GRAPH ATTRIBUTES:

RSPEC 6 9

NUMBER OF NODES IS 67

```
STEREO ATTRIBUTES: NONE
      322 SEA FILE=REGISTRY SUB=L3 SSS FUL L12
T. 1.4
```

L15 39 SEA FILE=CAPLUS SPE=ON ABB=ON PLU=ON L14 1 SEA FILE=CAPLUS SPE=ON ABB=ON PLU=ON L10 AND L15 L17 T-18 2 SEA FILE=CAPLUS SPE=ON ABB=ON PLU=ON L17 OR L10 L19 38 SEA FILE=CAPLUS SPE=ON ABB=ON PLU=ON L15 NOT L18

=> fil wpix

FILE 'WPIX' ENTERED AT 12:21:49 ON 24 DEC 2008 COPYRIGHT (C) 2008 THOMSON REUTERS

FILE LAST UPDATED: 22 DEC 2008 <20081222/UP> MOST RECENT UPDATE: 200882 <200882/DW> DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE >>> Now containing more than 1.2 million chemical structures in DCR <<<

>>> IPC Reform backfile reclassifications have been loaded to end of September 2008. No update date (UP) has been created for the reclassified documents, but they can be identified by 20060101/UPIC, and 20061231/UPIC, 20070601/UPIC, 20071001/UPIC, 20071130/UPIC, 20080401/UPIC, 20080701/UPIC and 20081001/UPIC. ECLA reclassifications to mid August and US national classification mid September 2008 have also been loaded. Update dates 20080401. 20080701 and 20081001/UPEC and /UPNC have been assigned to these. <<

FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE. PLEASE VISIT:

http://www.stn-international.de/training center/patents/stn guide.pdf

FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE http://scientific.thomsonreuters.com/support/patents/coverage/latestupdates/

EXPLORE DERWENT WORLD PATENTS INDEX IN STN ANAVIST, VERSION 2.0: http://www.stn-international.com/DWPIAnaVist2_0608.html

>>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

Page 2-A VAR G2=H/17/18/20/22/24/26/29/32/34 VAR G4=H/X/CN/NO2/45/46/48/49/NH2/52/55/COOH/57/61/63/64/66 NODE ATTRIBUTES: CONNECT IS E2 RC AT CONNECT IS X4 RC AT 19 CONNECT IS X4 RC AT 25 CONNECT IS X4 RC AT 28 CONNECT IS X4 RC AT 31 CONNECT IS E1 RC AT 33 CONNECT IS X4 RC AT 35 CONNECT IS X4 RC AT 39 CONNECT IS X4 RC AT CONNECT IS X4 RC AT 47 CONNECT IS X4 RC AT 48 CONNECT IS X4 RC AT 50

CONNECT IS E1 RC AT 53

```
CONNECT IS E1 RC AT 54
CONNECT IS E1 RC AT 56
CONNECT IS X4 RC AT 59
CONNECT IS X4 RC AT 62
CONNECT IS X5 RC AT 63
CONNECT IS E2 RC AT 64
CONNECT IS X4 RC AT 65
CONNECT IS E2 RC AT 66
CONNECT IS X4 RC AT 67
DEFAULT MLEVEL IS ATOM
GGCAT IS LOC UNS AT 17
GGCAT IS LOC SAT AT 19
GGCAT IS LOC SAT AT 25
GGCAT IS LOC SAT AT 25
GGCAT IS LOC SAT AT 28
GGCAT IS LOC SAT AT 31
GGCAT IS UNS AT 35
GGCAT IS LOC SAT AT 39
GGCAT IS LOC AT 45
GGCAT IS LOC SAT AT 47
GGCAT IS SAT AT 48
GGCAT IS LOC SAT AT 50
GGCAT IS LOC SAT AT 53
GGCAT IS LOC SAT AT 54
GGCAT IS LOC SAT AT 56
GGCAT IS LOC SAT AT 59
GGCAT IS LOC SAT AT 59
GGCAT IS UNS AT 62
GGCAT IS UNS AT 63
GGCAT IS SAT AT 64
GGCAT IS UNS AT 65
GGCAT IS SAT AT 66
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RSPEC 6 9
NUMBER OF NODES IS 67
STEREO ATTRIBUTES: NONE
L23
        17 SEA FILE=WPIX SSS FUL L12
L24
               3 SEA FILE=WPIX SPE=ON ABB=ON PLU=ON L23/DCR
=> dup rem 119 124
FILE 'CAPLUS' ENTERED AT 12:21:54 ON 24 DEC 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)
```

FILE 'WPIX' ENTERED AT 12:21:54 ON 24 DEC 2008 COPYRIGHT (C) 2008 THOMSON REUTERS PROCESSING COMPLETED FOR L19 PROCESSING COMPLETED FOR L24 T.34 39 DUP REM L19 L24 (2 DUPLICATES REMOVED) ANSWERS '1-38' FROM FILE CAPLUS ANSWER '39' FROM FILE WPIX

=> d 134 ibib abs hitstr tot

L34 ANSWER 1 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 1 ACCESSION NUMBER: 2006:845182 CAPLUS <u>Full-text</u> DOCUMENT NUMBER: 145:241713

TITLE: Antitumor agents containing benzoyl compounds INVENTOR(S):

Kanda, Yutaka; Soga, Shiro; Nakashima, Takayuki; Nara,

Shinji; Nakagawa, Hiroshi; Shiotsu, Yukimasa PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan

SOURCE:

PCT Int. Appl., 61pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent. LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO.											DATE							
	2006088193																		
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB	, BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,		
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ	, EC,	EE,	EG,	ES,	FI,	GB,	GD,		
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS	, JP,	KE,	KG,	KM,	KN,	KP,	KR,		
		KZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY	, MA,	MD,	MG,	MK,	MN,	MW,	MX,		
		MZ,	NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH	, PL,	PT,	RO,	RU,	SC,	SD,	SE,		
		SG,	SK,	SL,	SM,	SY,	TJ,	TM,	TN,	TR	TT,	TZ,	UA,	UG,	US,	UZ,	VC,		
		VN,	YU,	ZA,	ZM,	zw													
	RW	: AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE	, ES,	FI,	FR,	GB,	GR,	HU,	ΙE,		
		IS,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT	, RO,	SE,	SI,	SK,	TR,	BF,	ΒJ,		
		CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML	, MR,	NE,	SN,	TD,	TG,	BW,	GH,		
		GM,	KE,	LS,	MW,	ΜZ,	NA,	SD,	SL,	SZ	, TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,		
		KG,	ΚZ,	MD,	RU,	ΤJ,	TM												
													20060221						
C	A 259	9046			A1	2006	0824		CA:	2006-	2599	20060221							
El	2 185	2112			A1 20071107				EP 2006-714136						20060221				
	R:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE	, ES,	FI,	FR,	GB,	GR,	HU,	ΙE,		
											, PT,								
											2007-								
											2006-					0070	820		
	KR 2007104935															0070	913		
	IN 2007CN04135						2007	1116								0070			
PRIORI:	RIORITY APPLN. INFO.:										2005-								
											2006-					0060			
										WO :	2006-	JP30	2996		W 2	0060	221		
OTHER :	THER SOURCE(S):						145:	2417	13										

GI

Disclosed is a therapeutic agent for a tumor selected from a hematopoietic AB tumor and a solid tumor, comprising, as the active ingredient, a benzoyl compound represented by the general formula I or a prodrug or pharmacol. acceptable salt thereof: I wherein n is an integer of 1 to 5; R1 represents a substituted or unsubstituted lower alkoxy, a substituted or unsubstituted lower alkoxycarbonyl, CONR7R8 or the like; R2 represents a substituted or unsubstituted arryl or a substituted or unsubstituted aromatic heterocyclic group; R3 and R5 independently represent a hydrogen atom, a substituted or unsubstituted lower alkyl or the like; R4 represents a hydrogen atom, a halogen; and R6 represents a hydrogen atom, a halogen, a substituted or unsubstituted lower alkyl or the like. For example, the antitumor activity of a compound I (R1 = CON(CH2CH2OH)2; n = 1; R2 = p-methoxyphenyl; R3, R4, R5 = H; R6 = Et) was in vitro tested.

IT 819810-77-0

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(antitumor agents containing benzoyl compds.)

RN 819810-77-0 CAPLUS CN Methanone, [4,6-dib

Methanone, [4,6-dihydroxy-2-(2-methoxyethyl)[1,1'-biphenyl]-3-yl]phenyl-(CA INDEX NAME)

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 2 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 2 ACCESSION NUMBER: 2005:99354 CAPLUS Full-text

DOCUMENT NUMBER: 142:198068

TITLE: Preparation of aminopyrazoles as CHK1 checkpoint

protein kinase inhibitors.
INVENTOR(S): Johnson, Michael David; Teng, Min; Zhu, Jinjiang

PATENT ASSIGNEE(S): Pfizer Inc., USA SOURCE: PCT Int. Appl., 127 pp.

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT NO.				KIN	D	DATE			APPLICATION NO.						DATE			
WO	WO 2005009435				A1 20050203				WO 2	004-		20040714						
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,	
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,	
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,	
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	
		ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW	
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	
		ΑZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,	
		SI,	SK,	TR,	BF,	ΒJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	

SN, TD, TG						
CA 2532231	A1	20050203	CA	2004-2532231		20040714
BR 2004012820	A	20060926	BR	2004-12820		20040714
JP 2006528661	T	20061221	JP	2006-521691		20040714
US 20050043381	A1	20050224	US	2004-897849		20040722
MX 2006PA00933	A	20060330	MX	2006-PA933		20060124
PRIORITY APPLN. INFO.:			US	2003-489976P	P	20030725
			WO	2004-IB2397	W	20040714
OTHER SOURCE(S):	CASRE	ACT 142:1980	68: 1	MARPAT 142:198068		

AB Title compds. [I; L = 5-6 membered (substituted) heterocyclylene; Ar = 5-6 membered (substituted) (heterolaryl; R1 = (substituted) aryl(alkyl), heterocyclyl(alkyl), cycloalkyl(alkyl), alkenyl, alkyl; R2 = H, halo, (substituted) alkyl), were prepared Thus, title compound (II) (preparation outlined) inhibited human CHKl with Ki <1 nM.

IT 838823-36-2P 838823-58-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compound; preparation of aminopyrazoles as CHK1 checkpoint protein kinase inhibitors)

RN 838823-36-2 CAPLUS

GI

CN [1,1'-Biphenyl]-2,4-diol, 4'-[5-[[4-

[(cyclopropylamino)methyl]phenyl]amino]-1H-pyrazol-3-yl]-6-methyl- (CA INDEX NAME)

- RN 838823-58-8 CAPLUS
- CN [1,1'-Biphenyl]-2,4-diol, 6-methyl-4'-[5-[[4-[[(1methylethyl)amino]methyl]phenyl]amino]-1H-pyrazol-3-yl]- (CA INDEX NAME)

TТ 838824-28-59

> RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aminopyrazoles as CHK1 checkpoint protein kinase inhibitors)

- 838824-28-5 CAPLUS RN
- [1,1'-Biphenyl]-2,4-diol, 6-methyl-4'-[3-[[3-[[(1-

methylethyl)amino]methyl]phenyl]amino]-1H-pyrazol-5-yl]- (CA INDEX NAME)

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 3 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:14345 CAPLUS Full-text

DOCUMENT NUMBER: 142:93527

TITLE: Preparation of benzophenone derivatives as HSP90

inhibitors for treatment of tumor INVENTOR(S):

Nara, Shinji; Nakagawa, Hiroshi; Kanda, Yutaka;

Nakashima, Takayuki; Soga, Shiro; Kajita, Jiro; Saito,

Jun-ichi; Shiotsu, Yukimasa; Akinaga, Shiro

PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan

SOURCE: PCT Int. Appl., 206 pp.

CODEN: PIXXD2 DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

	PATENT NO.						KIND DATE				LICAT						
	WO 2005000778																
	W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB	, BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ	, EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS	, JP,	KE,	KG,	KP,	KR,	KZ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG	, MK,	MN,	MW.	MX,	MZ,	NA,	NI,
		NO.	NZ,	OM,	PG,	PH,	PL,	PT.	RO,	RU	, SC,	SD,	SE,	SG,	SK,	SL,	SY,
		TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US	, UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD	, SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
		AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM,	AT	, BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IT	, LU,	MC,	NL,	PL,	PT,	RO,	SE,
		SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM	, GA,	GN,	GQ,	GW,	ML,	MR,	NE,
		SN,	TD,	TG													
AU	2004	2519	49		A1 20050106				AU 2004-251949						2	20040	610
CA	2530	374			A1 20050106					CA :	2004-		20040610				
EP	1642	880			A1 20060405					EP :	2004-		20040610				
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR	, IT,	LI,	LU,	NL,	SE,	MC,	PT,
		IE,	SI,	FI,	RO,	CY,	TR,	BG,	CZ,	EE	, HU,	PL,	SK				
CN	1791	568			A		2006	0621		CN :	2004-	8001	3807		2	20040	610
US	US 20070032532					A1 2007020				US 2005-561415					2	0051	219
KR	KR 2006023576						2006	0314		KR :	2005-	7249	14		2	0051	226
PRIORIT	RIORITY APPLN. INFO.:									JP :	2003-	1854	75		A 2	20030	627
										WO :	2004-	JP84	94		N 2	0040	610
OTHER S	THER SOURCE(S):						MARPAT 142:93527										

GT

AB The title compds. I [wherein n = 1-10; R1 = H, OH, CN, etc.; R2 = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, or heteroaryl; R3 and R5 = independently H, (un)substituted alkyl, alkenyl, etc.; R4 and R6 = independently H, OH, halo, CN, etc.] or prodrugs or pharmaceutically acceptable salts thereof are prepared as heat-shock proteins (HSP) 90 inhibitors. For example, the compound II was prepared in a multi-step synthesis. II inhibited >30% human HSP90 at the concentration of 10 µM. I are useful as antitumor agents (no data).

IT 819810-77-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzophenone derivs. as $\ensuremath{\mathsf{HSP90}}$ inhibitors for

treatment of tumor)

RN 819810-77-0 CAPLUS

CN Methanone, [4,6-dihydroxy-2-(2-methoxyethyl)[1,1'-biphenyl]-3-yl]phenyl-(CA INDEX NAME)

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 4 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:651500 CAPLUS Full-text

DOCUMENT NUMBER: 143:302464

TITLE: Constituents of Vittaria anguste-elongata and Their

Biological Activities

AUTHOR(S): Wu, Pei-Lin; Hsu, Yu-Lin; Zao, Chen-Wei; Damu, Amooru

G.; Wu, Tian-Shung

CORPORATE SOURCE: Department of Chemistry, National Cheng Kung

University, Tainan, 701, Taiwan
SOURCE: Journal of Natural Products (2005), 68(8), 1180-1184

CODEN: JNPRDF; ISSN: 0163-3864

CODEN: JNPRDF; ISSN: U163-3864

PUBLISHER: American Chemical Society-American Society of Pharmacognosy

Journal

LANGUAGE: English

DOCUMENT TYPE:

OTHER SOURCE(S): CASREACT 143:302464

Twelve new compds., vittarin-A (1), -B (2), -C (3), -D (4), -E (5), -F (6), 3-O-acetylniduloic acid (7), Et 3-O-acetylniduloate (8), Me 4-O-coumaroylquinate (9), vittarilide-A (10), and -B (11), and vittariflavone (12), as well as 20 known compds. have been isolated from the whole plant of Vittaria angusteelongata. The structures of these compds. were determined by spectroscopic and chemical transformation methods. 5,7-Dihydroxy-3',4',5'-trimethoxyflavone (18) displayed moderate cytotoxicity against human lung carcinoma and central nervous system carcinoma cell lines with inhibition of 89 and 61% at a concentration of 58 μM, resp. Vittarilide-A (10) and -B (11) and Et 4-Ocaffeoylquinate (14) exhibited moderate DPPH radical scavenging activity with IC50 values of 91, 290, and 234 μM, resp.

IT 864512-88-9P, Vittarin E

RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(constituents of Vittaria anguste-elongata and their biol. activities)

RN 864512-88-9 CAPLUS

CN [1,1'-Biphenyl]-2,2',4,4'-tetrol, 6,6'-bis[2-(3,4-dimethoxyphenyl)ethyl](CA INDEX NAME)

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 5 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2004:202747 CAPLUS Full-text

DOCUMENT NUMBER: 142:176721

TITLE: Product subclass 2: one oxygen and one nitrogen or

phosphorus atom AUTHOR(S): Ulrich, H.

CORPORATE SOURCE: Guilford, CT, 06437, USA

SOURCE: Science of Synthesis (2004), 17, 55-115

CODEN: SSCYJ9

PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review. Methods for preparing six-membered heteroatoms containing two unlike heteroatoms selected from O, N, or P are reviewed including

cyclization, ring transformation, aromatization, and substituent modification. IT 4946-96-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of six-membered heteroatoms containing two unlike heteroatoms selected from O, N, or P via cyclization, ring transformation,

aromatization, and substituent modification)

RN 4946-96-7 CAPLUS

CN [1,1'-Biphenvl]-2,2',4,4'-tetrol, 6,6'-dimethyl- (CA INDEX NAME)

REFERENCE COUNT: 214 THERE ARE 214 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L34 ANSWER 6 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN

December 24, 2008

ACCESSION NUMBER: DOCUMENT NUMBER:

TITLE:

CORPORATE SOURCE:

2002:261182 CAPLUS Full-text 137:140357

Novel concepts in directed biarvl synthesis, 97. Atropo-enantioselective synthesis of the natural bicoumarin (+)-isokotanin A via a configurationally stable biaryl lactone

AUTHOR(S):

Bringmann, Gerhard; Hinrichs, Jurgen; Henschel, Petra; Kraus, Jurgen; Peters, Karl; Peters, Eva-Maria Institut fur Organische Chemie, Universität Wurzburg, Wurzburg, 97074, Germany

SOURCE: European Journal of Organic Chemistry (2002), (6), 1096-1106

CODEN: EJOCFK: ISSN: 1434-193X PUBLISHER . Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:140357

GI

AB The atropo-enantioselective total synthesis of the axially chiral bicoumarin (+)-isokotanin A (I) is described. Key steps were the formation of a configurationally stable seven-membered biaryl lactone and its kinetic resolution by atroposelective ring cleavage. The previous assignment of the absolute configuration (M-atropoisomer) of I (and its synthetic precursors) was confirmed by quantum chemical CD calcns. 21255-80-1P 54440-25-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and optical rotation of; atropoenantioselective synthesis of natural bicoumarin (+)-isokotanin A via configurationally stable biarvl lactone)

21255-80-1 CAPLUS RN

[1,1'-Biphenyl]-2,2',4,4'-tetrol, 6,6'-dimethyl-, (1S)- (9CI) (CA INDEX NAME)



54440-25-4 CAPLUS RN

[1,1'-Biphenyl]-2,2',4,4'-tetrol, 6,6'-dimethyl-, (1R)- (9CI) (CA INDEX CN NAME)



65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 7 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN 2000:722713 CAPLUS Full-text

ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE:

134:29229

Formal synthesis of both atropisomers of desertorin C and an example of chirality transfer from a biphenyl axis to a spiro center and its reverse

AUTHOR(S):

Baker, Robert W.; Kyasnoor, Rekha V.; Sargent, Melvyn V.; Skelton, Brian W.; White, Allan H.

CORPORATE SOURCE:

School of Chemistry, University of Sydney, Sydney, 2006, Australia

SOURCE:

Australian Journal of Chemistry (2000), 53(6), 487-506

CODEN: AJCHAS; ISSN: 0004-9425 CSIRO Publishing

PUBLISHER: DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S): GI

CASREACT 134:29229

In connection with the synthesis of 4,4',7,7'-tetramethoxy-5,5'-dimethyl-6,8'bicoumarin (desertorin C) in enantiopure form, the diastereomeric ratios of the products of the reactions between 2-isopropyloxy-6-methoxy-4methylphenylmagnesium bromide and (4S)-4-isopropyl-2-(2,3,5-trimethoxyphenyl)-

4,5-dihydrooxazole, between 2,4-dimethoxy-6-methylphenylmagnesium bromide and (4S)-4-isopropyl-2-(2,3-dimethoxy-5-methylphenyl)-4,5-dihydrooxazol, and between 2.4-dimethoxy-6-(t-butyldimethylsilyloxy)methylphenylmagnesium bromide and the oxazole (I) were explored. The major product of the last mentioned reaction was converted into (S,4S)-4-isopropyl-2-(2'-hydroxymethyl-4',6,6'trimethoxy-4-methyl-1,1'- biphenyl-6-yl)-4,5-dihydroxazole, the axial configuration of which was confirmed by single crystal X-ray structural determination The similar product (\$,4\$)-2-(2',4',6-trimethoxy-4,6'-dimethyl-1.1'-biphenvl-6-vl)-4.5- dihydrooxazole was converted into (S)-1-(2.4'.6'trimethoxy-4,6'-biphenyl- 2-yl)ethanone (II) which furnished (S)-1-(2', 4', 6-trimethoxy-4, 6'-dimethyl-1, 1'-biphenyl-2-yl)acetamide (43%) and (S)-2,7'-dimethoxy-3',5',6-trimethyl-spiro(cyclohexa-2,5-die ne-1,1'-(1H)isoindole]-4-one (III) (30%) on Schmidt rearrangement. III on reduction and methylation regenerated II. The methodol, of Lipschutz was adapted for the synthesis of both enantiomers of 1,1'-(2',4-dihydroxy-6,6'-dimethoxy-2,4'dimethylbiphenyl-3.3' -divl)bisethanone which constitutes a formal synthesis

IT 220556-23-0P 312263-57-3P

of both enantiomers of desertorin C.

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(formal synthesis of both atropisomers of desertorin C and an example of chirality transfer from a biphenyl axis to a spiro center and its

RN 220556-23-0 CAPLUS

CN Ethanone, 1,1'-[(1R)-2,4',6'-trihydroxy-6-methoxy-2',4-dimethyl[1,1'-biphenyl]-3,3'-diyl]bis-(9CI) (CA INDEX NAME)

RN 312263-57-3 CAPLUS

CN Ethanone, 1,1'-[(1R)-2,4',6,6'-tetrahydroxy-2',4-dimethyl[1,1'-biphenyl]3,3'-divl]bis- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

December 24, 2008

L34 ANSWER 8 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1998:776061 CAPLUS Full-text

DOCUMENT NUMBER: 130:182277

TITLE: A formal synthesis of both atropenantiomers of

desertorin C
AUTHOR(S): Kyasnoor, Rek

AUTHOR(S): Kyasnoor, Rekha V.; Sargent, Melvyn V.
CORPORATE SOURCE: Department of Chemistry, University of Western

Australia, Nedlands, 6907, Australia

SOURCE: Chemical Communications (Cambridge) (1998), (24),

2713-2714

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal

LANGUAGE: Journal English

OTHER SOURCE(S): CASREACT 130:182277

Asym. synthesis of both enantiomers of 1,1'-(2',4-dihydroxy-6,6'-dimethoxy-2,4'-dimethylbiphenyl-3,3'- diyl)bisethanone allows the formal synthesis of both enantiomers of desertorin C, i.e. 4,4',7,7'-tetramethoxy-5,5'-dimethyl-6,8'- bicoumarin.

229556-22-9P 220556-23-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(formal synthesis of both atropenantiomers of desertorin C)

RN 220556-22-9 CAPLUS

CN Ethanone, 1,1'-[(1S)-4,6,6'-trihydroxy-2'-methoxy-2,4'-dimethyl[1,1'-biphenyl]-3,3'-diyl]bis- (9CI) (CA INDEX NAME)

RN 220556-23-0 CAPLUS

CN Ethanone, 1,1'-[(1R)-2,4',6'-trihydroxy-6-methoxy-2',4-dimethyl[1,1'-biphenyl]-3,3'-diyl]bis- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT L34 ANSWER 9 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1996:601196 CAPLUS <u>Full-text</u>

DOCUMENT NUMBER: 125:269955 ORIGINAL REFERENCE NO.: 125:50305a

TITLE: The screening of Alternaria alternata and Alternaria solani for alternariol and alternariol methyl ether

toxigenicity strains

AUTHOR(S): Kuang, Kaiyuan; Shi, Shiying; Luo, Yi; Fong, Jianlin CORPORATE SOURCE: Inst. Plant Protection, Shanghai Acad, Agricultural

Scis., Shanghai, 201106, Peop. Rep. China SOURCE: Zhenjun Xuebao (1996), 15(2), 109-113

CODEN: ZHXUET; ISSN: 0256-1883

PUBLISHER: Kexue
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

96 Alternaria strains isolated from diseased rinds of wheat, potato and eggplant were screened for toxigenicity of alternariol (AOH) and its's Me ether (AME) by the growth inhibition of Bacillus mycoides. 48 Strains (50%) exhibited toxic effects on B. mycoides. Examined by HPLC, 13 among 18 strains with moderate to high toxicity produced AOH and AME. More A. solani strains were toxic, but A. alternata produces more toxin. The most productive A. alternata XA-8 and A. solani SA-10 strains produced 280 and 95.5mg/kg AOH, and 5140 and 94.3 mg/kg AME.

IT 182259-28-5P

RL: ADV (Adverse effect, including toxicity); BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation) (screening of Alternaria alternata and Alternaria solani for alternariol and alternariol Me ether toxicenicity strains)

RN 182259-28-5 CAPLUS

CN [1,1'-Bipheny1]-2-carboxylic acid, 2',3,4',5-tetrahydroxy-6'-methy1-, methyl ester (CA INDEX NAME)



L34 ANSWER 10 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1991:607611 CAPLUS Full-text

DOCUMENT NUMBER: 115:207611

ORIGINAL REFERENCE NO.: 115:35413a,35416a

TITLE: Novel concepts in directed biaryl synthesis. 4.

Diastereoselective ring opening of achiral bridged biaryls using chiral O- and N-nucleophiles: first

atropo-enantioselective synthesis of

acropo-enancioseieccive synchesis o

(-)-4,4'-bis(orcinol)

AUTHOR(S): Bringmann, Gerhard; Walter, Rainer; Ewers, Christian

L. J.

CORPORATE SOURCE: Inst. Org. Chem., Univ. Wuerzburg, Wuerzburg, D-8700,

Germany

SOURCE: Synlett (1991), (8), 581-3

10/584.234 December 24, 2008

CODEN: SYNLES; ISSN: 0936-5214 DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 115:207611

GI

The atropisomer-selective cleavage of the bridged biaryl I, which has no AR stereogenic element, is described. The directed ring opening of the lactone bridge is achieved with chiral O- or N- nucleophiles, i.e., by external asym. induction. The application of this novel process to the 1st atropoenantioselective synthesis of the constitutionally sym., known (-)-4,4'bis(orcinol) II is described.

ΙT 21255-80-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of) 21255-80-1 CAPLUS RN

CN [1,1'-Biphenyl]-2,2',4,4'-tetrol, 6,6'-dimethyl-, (1S)- (9CI) (CA INDEX NAME)

L34 ANSWER 11 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1992:112682 CAPLUS Full-text

DOCUMENT NUMBER: 116:112682

ORIGINAL REFERENCE NO.: 116:18931a.18934a

TITLE: Analysis of differential scanning calorimetric data

for reactive chemicals

AUTHOR(S): Ando, T.: Fujimoto, Y.: Morisaki, S.

CORPORATE SOURCE: Res. Inst. Ind. Saf., Minist. Labour, Kivose, Japan

SOURCE: Journal of Hazardous Materials (1991), 28(3), 251-80

CODEN: JHMAD9; ISSN: 0304-3894

DOCUMENT TYPE: Journal

LANGUAGE: English

Results of DSC measurements of reactive chems. are presented. Exothermic onset temps. (To) and heats of decomposition (O) for chems, were analyzed to see if it is possible to classify thermal hazards based on the factors. The

values of the 2 factors, which were widely and uniformly distributed, were independent of each other, based on statistical considerations. It is possible to classify and to predict the thermal hazards of reactive chems, by 2-dimensional representation in terms of To and Q. The reactive chems. were classified into 28 types according to the functional groups. The effects of sample cell type (pinhole cell and sealed cell) and cell material on DSC results are outlined.

139139-02-9

RL: PRP (Properties)

(thermal hazard of, estimation of, DSC in)

RN 139139-02-9 CAPLUS

[1,1'-Biphenvl]-2,4-diol, 6-methvl-4'-nitro- (CA INDEX NAME) CN



L34 ANSWER 12 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1985:592864 CAPLUS Full-text

DOCUMENT NUMBER: 103:192864

ORIGINAL REFERENCE NO.: 103:31000h,31001a

TITLE: Microbial transformation of olivetol by Fusarium

roseum

AUTHOR(S): McClanahan, Robert H.; Robertson, Larry W.

CORPORATE SOURCE:

Coll. Pharm., Ohio State Univ., Columbus, OH, 43210, USA

Journal of Natural Products (1985), 48(4), 660-3

CODEN: JNPRDF: ISSN: 0163-3864

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 103:192864

In a study of pathways of metabolism of cannabinoids by microorganisms, in which olivetol served as an exptl. model of the n-pentylresorcinol moiety, F. roseum appeared to metabolize only the aromatic portion of the mol. F. roseum Was capable of biotransforming olivetol to form metabolites both more and less polar than the starting material. After a time-course study indicated the optimal length of incubation, a prepare-scale fermentation was performed to isolate sufficient quantities of metabolites for structure determination Two metabolites of olivetol were isolated and identified as mono-Me olivetol and 2,2',4,4'-tetrahydroxy-6,6'-dipentylbiphenyl.

98985-63-8

SOURCE:

RL: FORM (Formation, nonpreparative)

(formation of, by Fusarium roseum, in biotransformation of olivetol)

RN 98985-63-8 CAPLUS

[1,1'-Bipheny1]-2,2',4,4'-tetrol, 6,6'-dipenty1- (CA INDEX NAME) CN

98985-64-92

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of) 98985-64-9 CAPLUS

RN [1,1'-Biphenv1]-2,2',4,4'-tetrol, 6,6'-dipentv1-, 2,2',4,4'-tetraacetate

(CA INDEX NAME)

L34 ANSWER 13 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1979:419739 CAPLUS Full-text

DOCUMENT NUMBER:

91:19739 ORIGINAL REFERENCE NO.: 91:3293a,3296a

TITLE:

The absolute configuration and optical rotation of ter- and quaterphenvl derivatives of orcin

AUTHOR(S): CORPORATE SOURCE: Hess, Heinrich; Musso, Hans Inst. Org. Chem., Univ. Karlsruhe, Karlsruhe,

ОН

D-7500/1, Fed. Rep. Ger. SOURCE:

Liebigs Annalen der Chemie (1979), (3), 431-7 CODEN: LACHDL; ISSN: 0170-2041

Journal DOCUMENT TYPE:

LANGUAGE: German GI

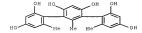
- The relative and absolute configuration of optical isomers of terphenyl AB derivs. I and quaterphenyl derivs. II, obtained from orcinol by oxidative coupling were determined
- 21255-80-1 54440-25-4
 - RL: RCT (Reactant); RACT (Reactant or reagent) (oxidative coupling of, with orcinol, configuration of optical isomers from)
- 21255-80-1 CAPLUS RN
- [1,1'-Bipheny1]-2,2',4,4'-tetrol, 6,6'-dimethyl-, (1S)- (9CI) (CA INDEX CN NAME)

- 54440-25-4 CAPLUS RN
- [1,1'-Bipheny1]-2,2',4,4'-tetrol, 6,6'-dimethyl-, (1R)- (9CI) (CA INDEX CN NAME)

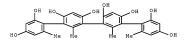
- IT 4946-96-7P 54440-26-5P 54440-29-8P
 - 54483-11-3P 54483-14-6P 54483-17-9P 54483-21-5P 67314-20-9P 67314-21-0P
 - 67314-22-1P 67314-23-2P 67314-24-3P 67314-25-4P

 - RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
- RN 4946-96-7 CAPLUS
- [1,1'-Biphenyl]-2,2',4,4'-tetrol, 6,6'-dimethyl- (CA INDEX NAME) CN

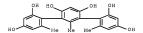
- RN 54440-26-5 CAPLUS



- RN 54440-29-8 CAPLUS
- CN [1,1':3',1'':3'',1'''-Quaterphenyl]-2,2''',4,4',4'',4''',6',6''-octol,
 2',2'',6,6'''-tetramethyl-, (R*,R*,R*)- (9CI) (CA INDEX NAME)



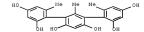
- RN 54483-11-3 CAPLUS



- RN 54483-14-6 CAPLUS
- CN [1,1':3',1'':3'',1'''-Quaterphenyl]-2,2''',4,4'',4''',6'',6'''-octol,
 2',2'',6,6'''-tetramethyl-, stereoisomer (9CI) (CA INDEX NAME)

- RN 54483-17-9 CAPLUS
- CN [1,1':3',1'':3'',1'''-Quaterphenyl]-2,2''',4,4',4'',4''',6',6''-octol,
 2',2'',6,6'''-tetramethyl-, (R*,S*,S*)- (9CI) (CA INDEX NAME)

RN 54483-21-5 CAPLUS



RN 67314-20-9 CAPLUS

CN [1,1':3',1'':3'',1'''-Quaterphenyl]-2,2''',4,4',4'',4''',6',6''-octol,
2',2'',6,6'''-tetramethyl-, stereoisomer (9CI) (CA INDEX NAME)

RN 67314-21-0 CAPLUS

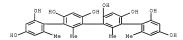
CN [1,1':3',1'':3'',1'''-Quaterphenyl]-2,2''',4,4',4'',4''',6'',6''-octol,
2',2'',6,6'''-tetramethyl-, stereoisomer (9CI) (CA INDEX NAME)

RN 67314-22-1 CAPLUS

CN [1,1':3',1'':3'',1'''-Quaterpheny1]-2,2''',4,4',4'',4''',6''-octol,
2',2'',6,6'''-tetramethy1-, stereoisomer (9CI) (CA INDEX NAME)

RN 67314-23-2 CAPLUS

CN [1,1':3',1'':3'',1'''-Quaterphenyl]-2,2''',4,4',4'',4''',6',6''-octol,
2',2'',6,6'''-tetramethyl-, stereoisomer (9CI) (CA INDEX NAME)



RN 67314-24-3 CAPLUS

CN [1,1':3',1'':3'',1'''-Quaterphenyl]-2,2''',4,4',4'',4''',6',6''-octol,
2',2'',6,6'''-tetramethyl-, stereoisomer (9CI) (CA INDEX NAME)

RN 67314-25-4 CAPLUS

CN [1,1:3',1':3'',1'''-Quaterpheny1]-2,2''',4,4',4'',4''',6',6''-octol,
2',2'',6,6'''-tetramethyl-, stereoisomer (9CI) (CA INDEX NAME)

L34 ANSWER 14 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1978:563181 CAPLUS Full-text

DOCUMENT NUMBER: 89:163181

ORIGINAL REFERENCE NO.: 89:25281a,25284a

TITLE: Complete separation of enantiomers by chromatography on potato starch

Hess, Heinrich; Burger, Guenther; Musso, Hans AUTHOR(S):

CORPORATE SOURCE: Inst. Org. Chem., Univ. Karlsruhe, Karlsruhe, Fed.

Rep. Ger.

SOURCE: Angewandte Chemie (1978), 90(8), 645-6 CODEN: ANCEAD: ISSN: 0044-8249

DOCUMENT TYPE: Journal

German

LANGUAGE:

Six enantiomeric mixts., e.q., (±)-6,6'-dinitrodiphenic acid and (±)-6,6'dimethyl-2,2',4,4'-biphenyltetrol, were completely separation by liquid chromatog, in a potato starch-filled column, using aqueous buffer solns, as eluents; the proper choice and concentration of buffer solution was important.

21255-80-1P 54440-25-4P 54440-26-5P 54483-11-3P 54483-21-5P 67314-20-9P 67314-21-0P 67314-23-2P 67314-24-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of) 21255-80-1 CAPLUS RN

[1,1'-Biphenyl]-2,2',4,4'-tetrol, 6,6'-dimethyl-, (1S)- (9CI) (CA INDEX CN

54440-25-4 CAPLUS RN

CN [1,1'-Biphenyl]-2,2',4,4'-tetrol, 6,6'-dimethyl-, (1R)- (9CI) (CA INDEX NAME)

54440-26-5 CAPLUS RN

CN [1,1':3',1''-Terphenvl]-2,2'',4,4',4'',6'-hexol, 2',6,6''-trimethyl-, (R*,R*)- (9CI) (CA INDEX NAME)

RN 54483-11-3 CAPLUS

CN [1,1':3',1''-Terpheny1]-2,2'',4,4',4'',6'-hexol, 2',6,6''-trimethyl-, (R*,S*)- (9CI) (CA INDEX NAME)

RN 54483-21-5 CAPLUS

RN 67314-20-9 CAPLUS

CN [1,1':3',1'':3'',1'''-Quaterphenyl]-2,2''',4,4',4'',4''',6',6''-octol,
2',2'',6,6'''-tetramethyl-, stereoisomer (9CI) (CA INDEX NAME)

RN 67314-21-0 CAPLUS

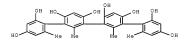
CN [1,1':3',1'':3'',1'''-Quaterphenyl]-2,2''',4,4',4'',4''',6''-octol,
2',2'',6,6'''-tetramethyl-, stereoisomer (9CI) (CA INDEX NAME)

RN 67314-23-2 CAPLUS

CN [1,1':3',1'':3'',1'''-Quaterphenyl]-2,2''',4,4',4'',4''',6',6''-octol,
2',2'',6,6'''-tetramethyl-, stereoisomer (9CI) (CA INDEX NAME)

RN 67314-24-3 CAPLUS

CN [1,1':3',1'':3'',1'''-Quaterphenyl]-2,2''',4,4',4'',4''',6',6''-octol,
2',2'',6,6'''-tetramethyl-, stereoisomer (9CI) (CA INDEX NAME)



IT 4946-96-7 54440-29-8 54483-14-6

67314-25-4

RL: PROC (Process)

(resolution of, by chromatog. on potato starch column) $4946-96-7\ \ \text{CAPLUS}$

RN 49

CN [1,1'-Biphenyl]-2,2',4,4'-tetrol, 6,6'-dimethyl- (CA INDEX NAME)

RN 54440-29-8 CAPLUS

CN [1,1':3',1'':3'',1'''-Quaterpheny1]-2,2''',4,4',4'',4''',6'',6''-octol,
2',2'',6,6'''-tetramethyl-, (R*,R*,R*)- (9CI) (CA INDEX NAME)

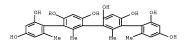
RN 54483-14-6 CAPLUS

CN [1,1':3',1'':3'',1'''-Quaterpheny1]-2,2''',4,4'',4'',4''',6',6''-octol,

2',2'',6,6'''-tetramethyl-, stereoisomer (9CI) (CA INDEX NAME)

RN 67314-25-4 CAPLUS

[1,1':3',1'':3'',1'''-Quaterphenyl]-2,2''',4,4',4'',4''',6',6''-octol, 2',2'',6,6'''-tetramethyl-, stereoisomer (9CI) (CA INDEX NAME)



L34 ANSWER 15 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1975:57470 CAPLUS Full-text

DOCUMENT NUMBER:

TITLE:

82:57470

ORIGINAL REFERENCE NO.: 82:9187a,9190a

Oxidation of orcinol with potassium hexacvanoferrate(III) in a flow system

AUTHOR(S): Haynes, Richard K.; Hess, Heinrich; Musso, Hans CORPORATE SOURCE: Inst. Org. Chem., Univ. Karlsruhe, Karlsruhe, Fed.

Rep. Ger. SOURCE: Chemische Berichte (1974), 107(12), 3733-48

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

GI For diagram(s), see printed CA Issue. AR

In contrast to static conditions oxidation of orcinol (I) by alkaline K3Fe(CN)6 in a flow system gave 35% dimer II (R = H) (III), smaller amts. of stereoisomeric trimers II [R = 6, 2, 4-Me(HO)2-C6H2] and stereoisomeric tetramers II [R = 3,2,4,6-R1Me(HO)2-C6H, R1 = 6,2,4-Me(HO)2C6H2] (IV) and practically no polymers. Similarly, III gave 50% mixture of all diastereomeric IV. The exclusive o,o'-coupling found in all products was related to the spin distribution of the unpaired electron in the radical of I.

4946-96-7P 54440-25-4P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(preparation and oxidation of)

(Reactant or reagent)

4946-96-7 CAPLUS RN

[1,1'-Bipheny1]-2,2',4,4'-tetrol, 6,6'-dimethyl- (CA INDEX NAME) CN



RN 54440-25-4 CAPLUS

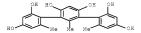
CN [1,1'-Bipheny1]-2,2',4,4'-tetrol, 6,6'-dimethyl-, (1R)- (9CI) (CA INDEX NAME)

IT 54440-26-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and resolution of)

RN 54440-26-5 CAPLUS

CN [1,1':3',1''-Terphenyl]-2,2'',4,4',4'',6'-hexol, 2',6,6''-trimethyl-, (R*,R*)- (9CI) (CA INDEX NAME)



- IT 54440-27-6F 54440-29-8F 54440-30-1F 54483-11-3F 54483-12-4F 54483-14-6F
 - 54483-15-7P 54483-17-9P 54483-18-0P

54483-21-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

(preparation of)

RN 54440-27-6 CAPLUS

CN [1,1':3',1''-Terphenyl]-2,2'',4,4',4'',6'-hexol, 2',6,6''-trimethyl-,
hexaacetate, (R*,R*)- (9CI) (CA INDEX NAME)

RN 54440-29-8 CAPLUS

CN [1,1':3',1'':3'',1'''-Quaterphenyl]-2,2''',4,4'',4''',6'',6''-octol,
2',2'',6,6'''-tetramethyl-, (R*,R*,R*)- (9CI) (CA INDEX NAME)

RN 54440-30-1 CAPLUS

RN 54483-11-3 CAPLUS

RN 54483-12-4 CAPLUS

CN [1,1':3',1''-Terphenyl]-2,2'',4,4',4'',6'-hexol, 2',6,6''-trimethyl-,
hexaacetate, (R*,S*)- (9CI) (CA INDEX NAME)

RN 54483-14-6 CAPLUS

CN [1,1':3',1'':3'',1'''-Quaterphenyl]-2,2''',4,4',4'',4''',6'',6''-octol,
2',2'',6,6'''-tetramethyl-, stereoisomer (9CI) (CA INDEX NAME)

RN 54483-15-7 CAPLUS

CN [1,1':3',1'':3'',1'''-Quaterphenyl]-2,2''',4,4',4'',4'',6'',6'''-octol,
2',2'',6,6'''-tetramethyl-, octaacetate, stereoisomer (9CI) (CA INDEX
NAME)

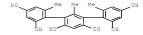
Aco

CN [1,1':3',1'':3'',1'''-Quaterphenyl]-2,2''',4,4'',4''',6',6'''-octol, 2',2'',6,6'''-tetramethyl-, (R*,S*,S*)- (9CI) (CA INDEX NAME)

RN 54483-18-0 CAPLUS

- RN 54483-21-5 CAPLUS
- CN [1,1':3',1''-Terphenyl]-2,2'',4,4',4'',6'-hexol, 2',6,6''-trimethyl-,

stereoisomer (9CI) (CA INDEX NAME)



L34 ANSWER 16 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1971:435291 CAPLUS Full-text

DOCUMENT NUMBER: 75:35291

ORIGINAL REFERENCE NO.: 75:5573a,5576a

TITLE: New synthesis of substituted arylquinones by means of electrophilic substitution of phenols, phenol ethers,

aromatic amines, and aromatic hydrocarbons by negatively substituted 1,4-benzoquinones

AUTHOR(S): Kuser, P.; Inderbitzin, M.; Brauchli, J.; Eugster, C.

CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, Switz.

SOURCE: Helvetica Chimica Acta (1971), 54(4), 980-95

CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal

LANGUAGE: German

AB Arylbenzohydroquinones and arylquinones, depending on the redox potential, were obtained together with 2-acetylbenzohydroquinone when 2-acetyl-1,4-benzoquinone (I) or 2-methoxycarbonyl-1,4-benzoquinone were treated with phenols, phenol ethers, amines, or hydrocarbons, in the presence of acid catalyst, preferably HOAc, H2CO2, F3CCO2H, or silica. Reaction of I with orcin gave 2-acetyl-3,3',6,6'-tetrahydroxy-2'- methylbiphenyl, which was oxidized to 2-acetyl-3-(2,4-dihydroxy-6-methylphenyl)-1,4-benzoquinone with Ag2O. 2-Acetyl-3-(4-methoxy-2-methylphenyl)-1,4-benzoquinone was obtained directly and intermediate isolation of the hydroquinone was not possible. Thirteen other hydroquinones and 23 quinones were similarly prepared

IT 32546-66-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 32546-66-0 CAPLUS

CN Ethanone, 1-(2',3,4',6-tetrahydroxy-6'-methyl[1,1'-biphenyl]-2-y1)- (CA INDEX NAME)



L34 ANSWER 17 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1972:2525 CAPLUS Full-text

DOCUMENT NUMBER: 76:2525 ORIGINAL REFERENCE NO.: 76:469a,472a derivatives as a preservative for sake

TITLE: Antiseptics for foods. LXXII. Diphenyl ether

derivatives, biphenyl derivatives, and dibenzofuran

AUTHOR(S): Fujikawa, Fukujiro; Hirayama, Teruhisa; Nakamura,

Yukio; Matsuo, Sachio; Mizutani, Takayuki; Mikawa, Toyoaki; Suzuki, Mitsuko; Doi, Mieko; Niki, Chiyo;

Toyota, Takeshi CORPORATE SOURCE: Kyoto Coll. Pharm., Kyoto, Japan

SOURCE: Yakugaku Zasshi (1971), 91(9), 930-3

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal LANGUAGE: Japanese

Antibacterial tests against Bacillus saprogenes, which causes putrefaction of sake, were carried out on 22 diphenyl ether compds., 2 dibenzofuran compds., and 4 biphenyl compds. In diphenyl ether compds., 4 compds. with an OH group in 1 benzene ring and a Me in the other benzene ring, such as 2-hydroxy-2'methyldiphenyl ether and 4-hydroxy-4'-methyldiphenyl ether, and a compound with a formyl and an OH in the same benzene ring, such as 4-formyl-2hydroxydiphenyl ether, had antibacterial activity 4-8-fold that of salicylic acid and 2-4-fold that of Bu p-hydroxybenzoate. Substitution of the Me group with carboxyl lowered the antibacterial activity. In biphenyl derivs., 2,2'and 4,4'-di-hydroxybiphenyl had antibacterial activity 8-fold that of salicylic acid and 4-fold that of Bu p-hydroxybenzoate. Increasing nos. of OH groups lowered antibacterial activity. In dibenzofuran compds., 3,7dihydroxydibenzofuran had twice the antibacterial activity of salicylic acid and was about comparable to Bu p-hydroxybenzoate. 3,7-Dihydroxy-1,9dimethyldibenzofuran increased the antibacterial activity to 8-fold that of salicylic acid and 4-fold that of Bu p-hydroxybenzoate, showing that increased Me groups resulted in stronger antibacterial activity.

4946-96-7

RL: BIOL (Biological study)

(Bacillus saprogenes inhibition by)

RN 4946-96-7 CAPLUS

CN [1,1'-Biphenvl]-2,2',4,4'-tetrol, 6,6'-dimethvl- (CA INDEX NAME)

L34 ANSWER 18 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1968:101679 CAPLUS Fuil-text

DOCUMENT NUMBER: 68:101679

ORIGINAL REFERENCE NO.: 68:19623a,19626a

TITLE: Chromatographic separation of antipodes of biphenyl derivatives

Steckelberg, Willi; Bloch, Michael; Musso, Hans AUTHOR(S):

CORPORATE SOURCE: Ruhr Univ. Bochum, Bochum, Fed. Rep. Ger. SOURCE: Chemische Berichte (1968), 101(4), 1519-21

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal LANGUAGE .

German

The title sepns. were carried out on potato starch with aqueous pH 7 buffer eluant, or on cellulose 21/2-acetate with benzene-AcOH eluant. OH, MeO, and Me-substituted, and quinonoid derivs. were separated

4946-96-7 RL: ANST (Analytical study)

(chromatog. and polarimetry of)

4946-96-7 CAPLUS RN

CN [1.1'-Biphenv1]-2.2',4.4'-tetrol, 6.6'-dimethyl- (CA INDEX NAME)

L34 ANSWER 19 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1968:115673 CAPLUS Full-text DOCUMENT NUMBER: 68:115673

ORIGINAL REFERENCE NO.: 68:22323a,22326a

TITLE:

SOURCE:

Orcein dyes. XXVI. Synthesis, configuration, and

spectra optical rotary dispersion-circular dichroism

of optically active orcein dyes

Musso, Hans; Steckelberg, Willi AUTHOR(S): CORPORATE SOURCE:

Ruhr Univ. Bochum, Bochum, Fed. Rep. Ger.

Chemische Berichte (1968), 101(4), 1510-18

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

Only the (R)(+)- β -components, β -hydroxyorcein, β -aminoorcein, and β aminoorceimine, were obtained from (R)(+)-2,4,6-

Me(MeO)(H2N)C6H2C6H2(NH2)(OMe)Me-2,4,6 via (R)(+)-2,4,6-

Me(HO)2C6H2C6H2(OH)2Me-2.4.6 indicating that the Me groups in the orcein

residue are trans in the β -component and cis in the γ -component. The Cotton effect of the long wavelength absorptions in these dyes is relatively weak, since the sym, phenoxazone chromophore is only made unsym, by the chiralic

bonding axes in the orcein residue. 18011-61-5P 21255-80-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 18011-61-5 CAPLUS

CN [1.1'-Biphenv1]-2.4.4'-triol, 2'-fluoro-6.6'-dimethyl- (CA INDEX NAME)

DM 21255-80-1 CAPLUS

[1,1'-Bipheny1]-2,2',4,4'-tetrol, 6,6'-dimethyl-, (1S)- (9CI) (CA INDEX CN

L34 ANSWER 20 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1968:21373 CAPLUS Full-text

DOCUMENT NUMBER: 68:21373

ORIGINAL REFERENCE NO.: 68:4071a,4074a

TITLE: Autoxidation rate and redox potential of hydroquinone,

pyrocatechol, and resorcinol derivatives AUTHOR(S): Musso, Hans; Doepp, Heinrike

CORPORATE SOURCE: Ruhr-Univ., Bochum, Fed. Rep. Ger.

SOURCE: Chemische Berichte (1967), 100(11), 3627-43

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

AB

The logarithm of the autoxidn, half-life time increased linearly with the redox potential for alkyl-substituted 1,4- and 1,3-C6H4(OH)2 and for alkylsubstituted 1,2,4-C6H3(OH)3.

4946-96-7 4947-12-0

RL: PRP (Properties) (autoxidn. and redox potential of)

RN 4946-96-7 CAPLUS

CN [1,1'-Biphenvl]-2,2',4,4'-tetrol, 6,6'-dimethyl- (CA INDEX NAME)

4947-12-0 CAPLUS

[1,1'-Bipheny1]-2,2',4,4',5-pentol, 6,6'-dimethyl- (CA INDEX NAME) CN



L34 ANSWER 21 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1967:54754 CAPLUS Full-text

DOCUMENT NUMBER: 66:54754

ORIGINAL REFERENCE NO.: 66:10299a,10302a

Oxidative condensation of catechols and resorcinols AUTHOR(S): Waiss, Anthony C., Jr.; Kuhnle, J. A.; Windle, John

J.; Wiersema, A. K.

CORPORATE SOURCE: Western Regional Res. Lab., U.S. Dep. of Agr., Albany,

CA, USA

Tetrahedron Letters (1966), (50), 6251-5 SOURCE:

CODEN: TELEAY; ISSN: 0040-4039 DOCUMENT TYPE: Journal English

LANGUAGE:

For diagram(s), see printed CA Issue.

cf. CA 60, 13119e. Equimolar (0.01M) solns. of 1,2,3(OH)2C6H3Pr-iso and 2,5-(HO) 2C6H3Me stirred with 1.0N NaOH in the presence of air rapidly turned green and gave a relatively stable (half-life >24 hrs.) free radical signal in the E.P.R. spectrum. The total extracted phenolic mixture treated with Me3SiSiMe3 and the product analyzed by vapor phase chromatography showed the presence of only one product (I, R = H) (II) and the hydrolyzate of the trimethylsilyl ether (I, R = SiMe3) (III) gave an E.P.R. peak identical with that of the main product II. III, C2504004Si3, λ 313, 303, 295, 259 mμ (C6H12) showed N.M.R. signals at t 8.63 d, 6.47 heptet (J 7.0), 3.53, 3.24 d (J 2.0), 7.39 s, 2.88 s. III heated with Ac20 and KOAc gave the corresponding acetate I (R = Ac), C22H22O7, m. 179-80°. The condensation was repeated in a limited supply of air, quenched with acid after 10 sec. and the trimethylsilyl ethers of the products analyzed by vapor phase chromatography to show the presence of 2 major product peaks corresponding to III and the trimethylsilyl ether (IV, R = SiMe3) (V) of the biphenyl derivative IV (R = H) (VI). Both V and the corresponding acetate IV (R = Ac) showed N.M.R. signals for 2 pairs of meta proton doublets, conclusively demonstrating the position of the C-C linkage in IV. The isolation of VI as an intermediate limits the structure of the dibenzofuran to I and an alternate (VII), which was excluded since the dibenzofuran gave a neg. Gibbs test. The E.P.R. spectrum of the radical anion of II consists of a quartet with intensity ratios 1:3:3:1 due to a hyperfine coupling to 3 equivalent protons with a coupling constant 1.22 oe. Each of these lines is split into a doublet by a single proton with a coupling constant 0.56 oe., and each of these is again split into 3 lines with intensity ratios 1:2:1 and coupling constant 0.13 oe., indicating coupling to 2 equivalent protons. The hyperfine couplings were assigned with the aid of deuterium analogs. The quartet was assigned to the Me group, the doublet to H-9, and the triplet to H-2 and H-4. No hyperfine coupling from the iso-Pr group was observed. The formation of dibenzofuran through mixed condensation reaction of catechols and resorcinols was found to be quite general though self-condensation was scarcely observed, if at all.

14253-45-3 RL: PRP (Properties)

(nuclear magnetic resonance of)

14253-45-3 CAPLUS RN

CN [1,1'-Bipheny1]-2,3',4,4'-tetrol, 6-methyl-5'-(1-methylethyl)-, 2,3',4,4'-tetraacetate (CA INDEX NAME)

14253-43-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

14253-43-1 CAPLUS RN

CN [1,1'-Biphenv1]-2,3',4,4'-tetrol, 6-methvl-5'-(1-methvlethvl)- (CA INDEX NAME)

L34 ANSWER 22 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1966:52506 CAPLUS Full-text DOCUMENT NUMBER: 64:52506

ORIGINAL REFERENCE NO.: 64:9846d-h,9847a-h

TITLE: Orcein dyes. XXV. Mechanism of formation and synthesis

of orcein dves AUTHOR(S): Musso, Hans; Zahorszky, Uwe Ingomar; Beecken, Hermann;

Gottschalk, Ellen Marie: Kraemer, Horst

CORPORATE SOURCE: Univ. Goettingen, Germany

SOURCE: Chemische Berichte (1965), 98(12), 3964-80

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal LANGUAGE: German

AB

For diagram(s), see printed CA Issue. GI

cf. preceding abstract The mechanism of the formation of orcein dyes was elucidated and a reaction scheme presented. Hydroxyhydroquinones react with NH3 via 4-aminoresorcinols to give tetrahydroxydiphenylamines which are readily oxidized by air to indophenols. The indophenols add in alkaline solution resorcinol derivs. and eliminate H2O with the formation of 2hydroxyphenoxaz-2-one derivs. β- and γ-Hydroxyorceins and hydroxyresorceins substituted on the chromophore and on the ring-substituents by Me groups were prepared according to this scheme. 1,2,4-C6H3(OH)3 (I) (100 mg.) in 20 cc. 1:1 NH4OHH2O heated 0.5 hr. at 50° and evaporated in vacuo, and the residue boiled 3 times with Et20 yielded from the extract 86.2 mg. light-gray, hygroscopic, air-sensitive product which was characterized as [2,4-(AcO)2C6H3]2NH (II). A similar run with 2,3,5-(HO)3C6H2Me yielded 2,4,6-Me(HO)2C6H2NH2 (III), isolated in 50% yield as [2.4.6-Me(AcO)2C6H212NH, m. 100°, 2.4-(HO)2.C6H3NH2.HCl (100 mg.) in a little H2O shaken in the absence of O with

about 1 q. Amberlite IR-4B (base) during 0.5 hr. yielded 63% viscous, light brown lacquer which was converted to II, m. 162°, [2,4-(HO)2C6H3]2NH (30 mg.), some AcONa, and 2 cc. Ac20 refluxed 0.5 hr., and the crude product chromatographed on Al203 vielded 12.2 mg. N-Ac derivative of II, m. 162°. III.HCl (6.0 q.) in 500 cc. H2O, 30 cc. N NaOH, and 100 cc. BuOH treated dropwise with stirring during 1.5 hrs. under N with 16.0 g. K3Fe(CN)6 in 500 cc. H2O and 20 cc. N NaOH and acidified, and 500 mg. of the residue (1.8 g.) from the BuOH phase chromatographed on silica gel yielded 200 mg. IV (R = Me, R' = OH, R'' = O). 2,3,4,6-Me(HO)3C6HC6H2(OH)2Me-2,4,6 (IVa) (100 mg.) treated under N with 10 cc. 1:1 NH4OH-H2O, purged 1 hr. with N, heated 6 hrs. at 100°, and evaporated, and the residue chromatographed on silica gel yielded 18 mg. β -V (R' = OH, R'' = O) (VI) [acetate, m. 138-40° (decomposition)] and 17 mg, v-V [acetate, m. 145-7° (decomposition)]. I (200 mg.) and 8.0 g. orcinol in 100 cc. H2O and 30 cc. 2N NH4OH kept 36 hrs. in air, and the product mixture chromatographed twice on cellulose powder yielded 90 mg. dark red VII, decompose at 350° without melting. Crude VII (200 mg.) acetylated and chromatographed gave 70 mg, orange pentaacetate of VII, m. 133-6°. III.HCl (400 mg.) and 8.0 g. m-C6H4(OH)2 in 170 cc. H2O and 10 cc. 2N NH4OH kept 3 days in air gave similarly 98 mg. dark red VIII, decompose at 350° without melting. VIII (30 mg.), some AcONa, and 2 cc. Ac20 heated 0.5 hr. on the water bath and chromatographed on silica gel gave 25 mg. orange pentaacetate of VIII, m. 129-32° (cyclohexane). III (109 mq.) in 5 cc. 1:1 C5H5N-Ac20 kept 24 hrs. at room temperature yielded 138 mg. 2,3,5-AcNH(AcO)2C6H2Me, m. 159° (CHCl3-C6H6), which was also obtained in 55% yield from III.HCl. III (128 mg.), 150 mg. AcONa, and 10 cc. Ac20 refluxed 3 hrs. and chromatographed on silica gel gave 198 mg. 2,3,5-Ac2N(AcO)2C6H2Me, m. 100.5° (C6H6-cyclohexane). 3,5,- 2,4-(HO)2(O2N)2C6HMe (214.1 mg.) in 3 cc. MeOH heated 1.5 hrs. with 1.489 g. SnCl2.2H2O in 3 cc. concentrated HCl and treated with H2S vielded 147.4 mg. 2,4,3,5-(H2N)2(HO)2C6HMe.2HCl (IX.2HCl). IX.2HCl (50 mg.) treated 24 hrs. at 20° with 4 cc. C5H5N-Ac2O gave 28.6 mg. 2,4,3,5-(AcNH)2(AcO)2C6HMe, m. 165-71° (C6H6-cyclohexane), IX.2HCL (100 mg.), 4 cc. Ac20, and 150 mg. Ac0Na refluxed 4 hrs. and poured into 30 cc. H2O gave 162 mg. 2,4,3,5-(Ac2N2)(AcO)2C6HMe (IXa), m. 137-8° (C6H6-cyclohexane). PhNH2 (3.726 g.) in 40 cc. 6N HCl diazotized with 3.0 q. NANO2 in 15 cc. H2O, diluted with iced H2O to 150°, and added dropwise during 25 min. to 5.686 q. 3,5-(HO)2C6H3Me.H2O and 30 g. AcONa in 3 l. H2O, and the product chromatographed on silica gel yielded 7.473 g. orange 2,3,5-PhN:N(HO)2C6H2Me (X), m. 195-6° (dioxanecyclohexane), and 632 mg. red 2,4,3,5-(PhN:N)2(HO)2C6HMe (XI), m. 234-5° (decomposition) (C6H6). X (247 mg.) treated at 60° with 600 mg. SnCl2 in 3 cc. concentrated HCl gave 185 mg. III.HCl which with Ac20-AcONa yielded 214 mg. 2,3,5-Ac2N(AcO)2C6H2Me, m. 98-9° (C6H6-cyclohexane). XI (333.6 mg.) gave similarly 188.7 mg. IX.2HCl which was converted to 92.5% IXa, m. 137-8°. PhNH2 (93.2 mg.) in 2 cc. 6N HCl diazotized with 70 mg. NaNO2 in 1 cc. H2O, diluted with 40 cc. iced H2O and added dropwise during 20 min. with stirring at 0° to 246.3 mg. [2,4,6-Me(HO)2C6H2]2 (XII), and the crude product (275.3 mg.) chromatographed on silica gel yielded 7 fractions of 34.6, 2.3, 16.8, 1, 81.3, 7.3, and 110.0 mg., resp. Fraction 7 gave the red 5-PhN:N derivative (XIII) of XII, m. 230-1° (decomposition); fraction 5 yielded the red 5,5'-bis(phenyiazo) derivative of XII, charring at 285-90° (C5H5N-AcOEt); and fraction 1 gave the dark red 3.5.5'-tris(phenylazo) derivative of XII, blackens above 200°: fraction 6 gave orange rhombs which were not investigated further. 2-Hydroxy-6-methyl-5-(2-methyl-4,6-dihydroxyphenyl)-p-benzoquinone (XIV) (0.2-0.25 q.) in 50 cc. C6H6 shaken with 1-2 g. In dust and 5 cc. AcOH until colorless gave light brown IVa, m. 217-20° (sublimed at 150° in vacuo); 1.66 g. XIV gave in this manner 1.05 g. IVa. XIII (50.7 mg.), 5 cc. MeOH, 5 cc. H2O, and 4 cc. concentrated HCl heated 3 hrs. on the water bath with 80 mg. ZnCl2, and the product refluxed 0.5 hr. with AcONa and 2 cc. Ac20 yielded 40.3 mg. 2,3,4,6-

December 24, 2008

Me(Ac2N)(AcO)2C6HC6H2(OAc)2Me-2,4,6 (XV), m. 133-4° (cyclohexane). IVa (100 mg.) in 10 cc. 1:1 NH4OH-H2O heated 7 hrs. under N on the water bath, and the crude product acetylated gave 113.7 mg. XV. The spectra of 7-hydroxy-2phenoxazone (XVI), the 4.5-dimethyl derivative of XVI, and 3.5-(HO)2C6H3Me between 300 and 700 mm are recorded.

- 4947-10-8P, 2.2', 4,4'-Biphenyltetrol, 6,6'-dimethyl-5-(phenylazo)-4947-12-0P, 2,2',4,4',5-Biphenylpentol, 6,6'-dimethyl-
 - 4947-13-1P, o-Diacetotoluidide, 3''-(4,6-dihydroxy-o-toly1)-4'',6''-dihydroxy-, tetraacetate
 - RL: PREP (Preparation) (preparation of)
- 4947-10-8 CAPLUS RN
- CN [1,1'-Biphenyl]-2,2',4,4'-tetrol, 6,6'-dimethyl-5-(2-phenyldiazenyl)- (CA INDEX NAME)

- RN 4947-12-0 CAPLUS
- [1,1'-Biphenv1]-2,2',4,4',5-pentol, 6,6'-dimethv1- (CA INDEX NAME) CN

- 4947-13-1 CAPLUS RN
- CN Acetamide, N-acetyl-N-[2',4,4',6-tetrakis(acetyloxy)-2,6'-dimethyl[1,1'biphenyl]-3-yl]- (CA INDEX NAME)

- ACCESSION NUMBER: DOCUMENT NUMBER:
- L34 ANSWER 23 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN 1966:52505 CAPLUS Full-text 64:52505

10/584,234 December 24, 2008

ORIGINAL REFERENCE NO.: 64:9845f-h,9846a-d

TITLE: Orcein dyes. XXIV. Mechanism of autoxidation of resorcinol derivatives

AUTHOR(S): Musso, Hans; Gizycki, Ulrich v.; Kraemer, Horst;

Doepp, Heinrike
CORPORATE SOURCE: Univ. Goettingen, Germany

SOURCE: Chemische Berichte (1965), 98(12), 3952-63

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal LANGUAGE: German

GI For diagram(s), see printed CA Issue.

cf. CA 64, 8351d. The mechanism by which 1,3,5-MeC6H3(OH)2 (I) is oxidized in AR alkaline solution by atmospheric O to the dimeric quinones II and III was investigated by isolating intermediates chromatographically, by kinetic measurements, and by preparative studies with sterically hindered model compds. I.H2O (5.1 g.) and 3.6 g. KOH in 85 cc. H2O, treated with stirring under N dropwise during 3.5 hrs. with 29.0 g. K3Fe(CN)6 in 80 cc. H2O and acidified with 2N H2SO4, and the precipitate (2.8 g.) repptd. from EtOH with 2N H2SO4, gave the polymeric IV; the acidified filtrate extracted with BuOH, and the extract chromatographed on paper showed the presence of I, [2,4,6-Me(HO)2C6H2]2 (V), IV, and 4 phenolic compds. IV (500 mg.), 500 mg. Na, and 10 cc. dry C5H5N refluxed 6 hrs. under N, treated successively with 10 cc. 1:1 aqueous C5H5N and 10 cc. H2O, acidified with 50% H2SO4, and extracted with BuOH gave 57 mg. product mixture; the H2O-soluble portion of the mixture (40 mg.) sublimed at 120-80° in vacuo gave 8 mg. mixture of I and V. I. (1.0 g.) and 2.0 g. BzPh in 200 cc. C6H6 under N irradiated with an immersed 125-w. uv lamp during 5 hrs. gave 830 mg. colorless solid and 1.0 g. BzPh; 2.0 g. colorless product chromatographed on cellulose powder, and the main product sublimed at $150-70^{\circ}$ in vacuo yielded 40 mg. V, m. 232° (CHC13). VI (R = Me) (198 mg.) and 2 g. dry C5H5N.HCl heated 2.5 hrs. at 180° under N gave 160 mg. (crude) hydroscopic VI (R = H) (VII), m. 80-1°, Crude VII (46 mg.), 1 cc. Ac20, and 1 cc. C5H5N kept 3 hrs. at room temperature yielded 34.7 mg. 2,4,6-Me(AcO)2C6H2OC6H3(OAc)Me-3,5 (VIII), m. 81° (cyclohexane), VII (160 mg.), 80 cc. H2O, and 20 cc. 0.2M K2HPO4 treated at 0° with stirring with 540 mg. NO(SO3K)2 in 40 cc. 0.2M K2HPO4, acidified after 1 hr. with 2N H2SO4, and extracted with BuOH, and the residue from the extract (160 mg.) chromatographed on cellulose powder yielded some II and 20 mg. orange-brown IX, m. 137-9° (decomposition) (C6H6). IX (100 mg.), 2 g. Zn dust, and 0.5 g. AcONa in 10 cc. Ac20 refluxed until colorless gave 89 mg. 5-AcO derivative of VIII. The comparative autoxidn. of I and V demonstrated that V was oxidized nearly 10 times as fast as I. If the autoxidn, of I and V is performed in the presence of K3Fe(CN)6, in order to produce free ordinol radicals which are consumed immediately, the presence of V can be demonstrated chromatographically in the mixture, proving that V is not an intermediate in the oxidation of I to II and III. The autoxidn. of V proceeded without the formation of H2O2.

IT 4946-96-7P, 2,2',4,4'-Biphenyltetrol, 6,6'-dimethyl-RL: PREP (Preparation)

(preparation of)

RN 4946-96-7 CAPLUS

CN [1,1'-Bipheny1]-2,2',4,4'-tetrol, 6,6'-dimethyl- (CA INDEX NAME)



L34 ANSWER 24 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1964:492144 CAPLUS Full-text

DOCUMENT NUMBER: 61:92144

ORIGINAL REFERENCE NO.: 61:16008a-h

TITLE: Formation of hydroxy aryl quinones by the addition of phenols to quinones

AUTHOR(S):

Musso, Hans; Gizycki, Ulrich v.; Zahorszky, Uwe I.;

Bormann, Dieter

CORPORATE SOURCE: Univ. Marburg, Germany

SOURCE: Justus Liebigs Annalen der Chemie (1964), 676, 10-20

CODEN: JLACBF; ISSN: 0075-4617

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 61:92144 For diagram(s), see printed CA Issue. AB

Resorcinol derivs. add in alkaline solution to hydroxyquinones to yield the corresponding dihydroxyarylhydroguinones. PHOH reacts in acidic and alkaline solution with p-benzoquinone (I) to give o-(II) and phydroxyphenylbenzoguinone (III); in neutral solution phenoxyguinones are also formed. The condensation of hydroxy-p-xyloquinone (IV) with BF3 led to a dibenzofuranquinone, present in nonpolar solvents as diphenoquinone. m-C6H4(OH)2 (1 g.) in 25 cc. 0.2M phosphate buffer (pH 12) and 4 cc. 2N NaOH treated dropwise with stirring in air with 100 mg. 1,2,4-C6H3(OH)3 in 10 cc. H2O and acidified after 20 min. with dilute H2SO4, and the crude product chromatographed on silica gel yielded 38 mg. V (R = R1 = R2 = R3 = H) (VI), dark brown needles, blacken up to 320° without melting. Similarly were prepared the following V (R, R1, R2, R3, % yield, and m.p. given): Me, H, Me, H, 92.5, 182-7° (decomposition); Me, Me, Me, Me, 90, 224-5°; tert-Bu, H, tert-Bu, H, 39.5, 225-7° (orange needles) (AcOEtcyclohexane); H, H, Me, H, 28, 190-200° (decomposition); Me, H, H, H, 11, 180-200° (decomposition). VI (125 mg.) in 5 cc. Ac2O heated 0.5 hr. on the water bath with NaOAc and In dust, and the product chromatographed on silica gel yielded 207 mg. 2,2',4,4',5pentaacetoxybiphenyl (VII), m. 123-4° (cyclohexane-C6H6). Similarly were prepared the following derivs. of VII (substituent, % yield, and m.p. given): 6'-Me, 68, 136-9°; 6-Me, 84, 133-4°. 6-Hydroxytoluhydroquinone (141 mg.) in 25 cc. 0.2M phosphate buffer (pH 12) stirred 1 hr. in air and acidified with dilute H2SO4, and the product chromatographed on silica gel yielded 91 mg. 4,4'-dihydroxy-2,2'-ditolyldiquinone, yellow needles, m. 207°. Similarly was prepared 4,4'-dihydroxy-3,3',6,6'- tetramethylbiphenyldiquinone, 68%, m. 208-10°. PhOH (5.64 g.) and 1.58 g. KOH in 20 cc. H2O treated with stirring with 0.648 g. I in 20 cc. H2O and acidified after 4 min. with dilute H2SO4, and the product chromatographed on silica gel yielded 5 mg. 5-PhO derivative (VIII) of 2-(p-hydroxyphenoxy)-1,4-benzoquinone (IX), light yellow needles, m. 224-6°, and 43 mg. III, m. 177° (C6H6-cyclohexane). PhOH (5.64 g.) in 35 cc. 20% H2SO4 and 7 cc. MeOH treated 0.5 hr. at 40° with 0.65 g. I vielded 103 mg. II, m. 192-3°, and 10 mg. III. I (3q.) and 18 q. PhOH in 850 cc. H2O and 150 cc.

MeOH kept 20 days, and the crude product chromatographed on silica gel yielded 170 mg. yellow 2,5-diphenoxy-1,4-benzoquinone, m. 236-7° (cyclohexane), 95 mg. X, 220 mg. IX, 100 mg. VIII, yellow needles, m. 224-6° (AcOEt-cyclohexane), and 1.5 g. p-C6H4(OH)2. VIII (20 mg.) with 5 cc. Ac20 and 1 cc. C5H5N yielded 17 mg. acetate of VIII, vellow-green needles, m. 192-4° (C6H6). VIII (27 mg.) in 10 cc. Ac20 treated with 2 q. Zn dust yielded 22 mg. 2-(p-acetoxyphenoxy)-5-phenoxyhydroquinone diacetate, m. 102° (C6H6-cyclohexane). I (2 g.) in 200 cc. H2O and 25 cc. MeOH kept 9 days and acidified with dilute H2SO4 yielded 25 mg. IX, vellow needles, m. 145-6° (C6H6-cyclohexane). IX (216 mg.) and 2 g. PhOH in 150 cc. H2O and 25 cc. MeOH kept 13 days yielded 25 mg. VIII, yellow needles, m. 224-6° (AcOEt-cyclohexane). II (100 mg.) in 30 cc. dry Et20 treated 2 hrs. with 0.5 cc. Et20.BF3 yielded 80 mg. 1,4,5,8-tetramethyl-3,6dihydroxydibenzofuran-2,7-quinone (XI), black-blue needles, decompose slowly above 300° without melting up to 350° (AcOEt). II (150 mg.) in 15 cc. AcOH treated 4 hrs. at room temperature with 0.5 cc. concentrated H2SO4 gave 102 mg. XI. XI (100 mg.) and a small amount NaOAc in 5 cc. Ac2O heated with the portionwise addition of 3 g. In dust until the mixture was colorless gave 116 mg. 1,4,5,8-tetramethyl-2,3,6,7-tetraacetoxydibenzofuran (XII), needles, m. 275-6° (C6H6). 2,7-Dihydroxy-4,5-dimethyldibenzofuran (30 mg.) in 10 cc. Ac20 and 1 cc. C5H5N heated 15 min. on the water bath, and the crude product chromatographed on silica gel yielded 34 mg. diacetate, needles, m. 181-2° (C6H6-cyclohexane). XI (100 mg.) in 100 cc. Me2CO and 5 cc. 2N HCl shaken with Zn dust until colorless gave 30 mg. 2,3,6,7-tetra-OH analog (XIII) of XII, needles, m. 285-300° (decomposition). The ultraviolet spectra of XI and XIII are recorded.

IT 104667-25-6P, 2,2',4,4',5-Biphenylpentol, 6-methyl-, pentaacetate 107893-61-8P, 2,2',4,4',5-Biphenylpentol, 6'-methyl-, pentaacetate RL: PREP (Preparation)

(preparation of) RN 104667-25-6 CAPLUS

CN [1,1'-Biphenyl]-2,2',4,4',5-pentol, 6-methyl-, 2,2',4,4',5-pentaacetate
 (CA INDEX NAME)

RN 107893-61-8 CAPLUS

CN [1,1'-Bipheny1]-2,2',4,4',5-pentol, 6'-methyl-, 2,2',4,4',5-pentaacetate
(CA INDEX NAME)

10/584,234 December 24, 2008

ACCESSION NUMBER: 1963:436058 CAPLUS Full-text

DOCUMENT NUMBER: 59:36058

ORIGINAL REFERENCE NO.: 59:6546h,6547a-h,6548a-e

TITLE: Orcein pigments. XX. The autoxidation products of 2.5-dimethylresorcinol in ammonia and potassium

hydroxide

AUTHOR(S): Musso, Hans; Zahorszky, Uwe I.

CORPORATE SOURCE: Univ. Marburg, Germany

SOURCE: Chemische Berichte (1963), 96, 1593-1609

CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal

LANGUAGE:

Unavailable

GI For diagram(s), see printed CA Issue.

AB The autoxidn. of 2,5,1,3-Me2(HO)2C6H2 (I) in NH4OH yielded dyes analogous to

those obtained from 3,5-(HO)2C6H3Me (II). The autoxidn. in aqueous KOH vielded, in addition to the dimeric mono- and diguinone, a trimeric diguinone which could not be identified with certainty in the product from II. The autoxidn. of I proceeds faster and furnishes better yields of the higher oxidized products which are more stable than those from II. I (14 g.) in 140 cc. concentrated NH4OH kept 25 days at room temperature in air while being treated daily with dry NH3 during a few min., concentrated in vacuo over concentrated H2SO4, and dried over P2O5 yielded 16.8 g. crude, violet-black, amorphous powdery xylorcein which, extracted at about 70° with the upper phase of 5:1:2.6:5 C6H6-BuOH-AcOH-H2O and then chromatographed on cellulose powder, yielded 0.46 g. III (R = OH) (IV), red-brown crystals, m. 340° (decomposition) (MeOH-CHCl3), 0.85 g. (crude) trans-V (R = OH) (VI) (the OH groups on the benzene rings are in the trans configuration with respect to the phenoxazone plane), red-brown crystals, m. 280° (MeOH-CHCl3), 0.94 g. (crude) cis-V (R = OH) (VIA), red-brown crystals, m. 280° (decomposition), 0.35 g. (crude) III (R = NH2) (VII), red rodlets, m. 370° (decomposition) (MeOH-CHCl3), 0.90 g. (crude) trans-VIII (R = 0) (IX) rodlets with a green-black luster, m. 300° (decomposition), 1.30 g. (crude) cis-VIII (R = 0), (IXA), green-black glistening rodlets, m. 350° (decomposition), 0.26 g. trans-X (XI), green-black glistening crystals, m. 350° (decomposition) (MeOH-CHCl3), 0.38 g. (crude) cis-X, green-black needles, m. 350° (decomposition) (MeOH-CHCl3), 0.35 g. (crude) cis-VIII (R = NH) (XII), and 0.25 q. (crude) trans-VIII (R = NH) (XIIA). IV (50 mg.) in 5 cc. dry C5H5N treated at room temperature with 5 cc. Ac20, evaporated after 24 hrs., and the residue chromatographed on silica gel yielded 26 mg. red triacetate B of IV, m. 222-5° (decomposition) (C6H6cyclohexane), and 7 mg. triacetate A of IV, yellow needles, m. 234-7° (decomposition). VI (100 mg.) gave similarly 15.9 mg. orange triacetate of VI, m. 240° (decomposition) (C6H6-cyclohexane). VI (52 mg.) in 20 cc. EtOH warmed 5 hrs. on the water bath with 250 mg. o-C6H4(NH2)2 (XIII) in 10 cc. AcOH and evaporated, and the residue evaporated with C5H5N and chromatographed on silica gel yielded 20 mg. phenazine derivative of VI, orange crystals, m. 231-3° (decomposition) (C6H6-cvclohexane). VIA (43 mg.) treated 24 hrs. with Ac20-C5H5N at room temperature and evaporated, and the residue chromatographed on CaSO4 yielded 21 mg. triacetate of VIA, orange-yellow crystals, m. 239-42° (decomposition). VIA (77 mg.) and XIII yielded 16.5 mg. yellow phenazine derivative, m. 213-17° (decomposition) (C6H6-cyclohexane). VII (120 mg.), Ac20, and NaOAc refluxed 20 min., and the crude product chromatographed successively on silica gel and CaSO4 yielded 10.5 mg. red triacetate of VII, m. 160-3° (decomposition). IX (139 mg.) acetylated and chromatographed on silica qel qave 34 mg. N-Ac tetraacetate derivative of IX, red rodlets, m. 165-70° (decomposition). IXA (96 mg.) acetylated with Ac20-NaOAc and chromatographed on CaSO4 yielded 21 mg. N-Ac tetraacetate derivative of IXA, orange-red crystals, m. 172-5° (decomposition). XI (30 mg.) with C5H5N-Ac20 vielded during 3 days at room temperature 13 mg. N-Ac triacetate derivative of

XI, orange crystals, m. 164-7° (decomposition) (C6H6-cyclohexane), cis-X (55 mg.) yielded similarly 13.9 mg. N-Ac triacetate derivative of cis-X, redorange crystals, m. 172-5° (decomposition) (C6H6-cyclohexane). Crude XII (160 mg.) or 120 mg. XIIA were repptd. from a few cc. MeOH with C6H6 and filtered, and the blue amorphous residues, which did not melt up to 340° but decomposed with effervescence when inserted at 240°, were isolated as XII.1/2H2SO4 and XIIA.1/2H2SO4.MeOH, resp. Pure VI or VIA (1 mg.), each in 1 cc. glycerol heated in vacuo in a sealed tube at 185° and partitioned after 1 hr. between BuOH-H2O, and the residues from the red BuOH phases chromatographed on cellulose powder showed that both dyes were isomerized to about 50%. IX and IXA heated to 200° during 1 hr. turned red-brown; in glycerol during 1.5 hrs. at 200° only brown-black decomposition products were formed. I (10 g.) and 8.6 q. KOH in 200 cc. H2O kept 5 days at room temperature in the air, acidified with dilute H2SO4, and extracted with BuOH vielded 8.6 g. dark brown mass which dissolved in 100 cc. upper phase of BuOH-0.2M phosphate buffer (pH 7) and chromatographed on cellulose powder yielded 2.2 g. 6-hydroxy-2,5dimethyl-3-(4,6-dihydroxy-2,5-dimethylphenyl)-1,4- benzoquinone (XIV), red rodlets, m. 223-4° (MeOH CHCl3), 60 mg. 2,5-dimethvl-4,6-bis(4-hvdroxv-3,6dioxo-2,5-dimethyl-1,4- cyclohexadienyl)resorcinol (XV), orange rodlets, m. 282-3° (MeOH), pK 6.80, and 752 mg, 4,4'-dihydroxy-3,6,3'6'tetramethylbiphenyl-2,5,2',5'- diquinone (XVI), orange-yellow rhombs, m. 208-10° (MeOH and sublimed in vacuo at 170°). XIV (195 mg.) in 5 cc. C5H5N and 5 cc. Ac20 evaporated after 0.5 hr. and chromatographed on silica gel yielded 197 mg. triacetate of XIV, yellow crystals, m. 156-7° (C6H6-cyclohexane). XIV (245 mg.), 5 cc. Ac20, and a little NaOAc refluxed 5 min. while being treated with Zn dust in small portions and evaporated yielded 380 mg. 3,4,6,4',6'pentaacetoxy-2,5,2',5'- tetramethylbiphenyl, m. 182-3° (C6H6-cyclohexane). XIV (175 mg.) and 200 mg. XIII in 4 cc. AcOH heated 0.5 hr. on the water bath and evaporated, and the residue chromatographed on silica gel yielded 150 mg. phenazine derivative (XVII), yellow-green crystals, m. 259-60° (EtOH-C6H6). XVII (120 mg.) acetylated with 5 cc. C5H5N and 5 cc. Ac2O, and the product chromatographed on silica gel yielded 118 mg. triacetate of XVII, yellow-brown crystals, m. 200-2° (EtOH). XV (14.4 mg.) in 5 cc. Ac20 refluxed 5 min. with a small amount NaOAc while being treated with Zn dust in small portions, and the product chromatographed on silica gel gave 13.2 mg. 3,5-diacetoxy-2,6bis(3,4,6-triacetoxy-2,5- dimethylphenyl)-p-xylene, m. 204-5° (C6H6cyclohexane). XVI (113 mg.) yielded similarly 109 mg. yellow diacetate of XVI, m. 142-3° (C6H6-cyclohexane). XVI (86 mg.) acetylated reductively vielded 126 mg. [2,5,3,4,6-Me2(AcO)3C6]2, m. 188-90° (C6H6-cyclohexane). XVI (47 mg.) and 150 mg. XIII in 5 cc. AcOH heated 0.5 hr. on the water bath, and the product chromatographed on silica gel vielded 20 mg. phenazine derivative (XVIII), black-blue needles, m. 229-31° (EtOH). XVIII (200 mg.) in 3 cc. C5H5N treated with 5 cc. Ac2O and evaporated immediately in vacuo and the residue chromatographed on silica gel yielded 94 mg. 3,3'-diacetoxy-1,4,1',4'tetramethyl-2,2'-biphenazine, pale yellow, m. 299-300° (C6H6-cyclohexane). The infrared absorption maximum of the various compds. described and the ultraviolet absorption maximum of the various quinone are tabulated. 4946-96-7, 2,2',4,4'-Biphenvltetrol, 6,6'-dimethyl-

(spectrum of) RN 4946-96-7 CAPLUS

IT

CN [1,1'-Biphenv1]-2,2',4,4'-tetrol, 6,6'-dimethv1- (CA INDEX NAME)



L34 ANSWER 26 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN 1963:436057 CAPLUS Full-text ACCESSION NUMBER:

DOCUMENT NUMBER: 59:36057

ORIGINAL REFERENCE NO.: 59:6546e-h

TITLE: Orcein pigments. XIX. The effect of ortho-methyl

groups on the electronic spectra and pK values of orcein dyes and hydroxybiphenyl derivatives

AUTHOR(S): Musso, Hans; Zahorszky, Uwe I.

CORPORATE SOURCE: Univ. Marburg, Germany

SOURCE: Chemische Berichte (1963), 96, 1588-92

CODEN: CHBEAM; ISSN: 0009-2940 DOCUMENT TYPE: Journal

LANGUAGE:

Unavailable GI For diagram(s), see printed CA Issue.

AB The striking difference in the absorption spectra and pK values between

resorcinol blue and orcein dyes is explained by steric resonance hindrance and H bonds and confirmed on colorless tetrahydroxybiphenvl derivs. The pK values are given for the following compds.: I (R = OH, R' = H)6.40; I (R = OH, R' = Me) 6.76; II (R = OH, R' = H) 5.31; II (R = OH, R' = Me) 4.64; III (R = OH, R' = H, R'' = Me) 7.15; III (R = OH, R' = Me, R'' = H) 7.35; IV (R = OH) 7.46. The ultraviolet absorption spectra of [2,4(HO)2C6H3]2, [4,2,6-Me(HO)2C6H2]2, 2,4-(HO)2C6H3Me, 1,4,3,5Me2(HO)2C6H2, 1,2,3,5-Me2(HO)2C6H2, and [2,4,6-Me(HO)2C6H2]2 are recorded.

4946-96-7, 2,2',4,4'-Biphenyltetrol, 6,6'-dimethyl-

(spectrum of)

RN 4946-96-7 CAPLUS

CN [1,1'-Biphenyl]-2,2',4,4'-tetrol, 6,6'-dimethyl- (CA INDEX NAME)

L34 ANSWER 27 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1961:71148 CAPLUS Full-text

DOCUMENT NUMBER: 55:71148

ORIGINAL REFERENCE NO.: 55:13536c-f

TITLE: Biosynthesis of fungal metabolites. II. The

biosynthesis of alternariol and its relation to other

fungal phenols

AUTHOR(S): Thomas, R. CORPORATE SOURCE: Univ. London

SOURCE: Biochemical Journal (1961), 78, 748-58

CODEN: BIJOAK; ISSN: 0264-6021

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

cf. CA 54, 22821q. The biosynthesis of alternariol (I), C14H10O5, from Alternaria tenuis has been studied. Chemical degradation of labeled I derived from AcONa-1-C14 (CA 48, 799i) demonstrated a biosynthetic mechanism involving head-to-tail condensation of Aco units. I was methylated to the tri-Me ether with Me2SO4 and K3CO2 in anhydr, acetone by refluxing the mixture Kuhn-Roth oxidation of the trimethyl ether derivative yielded AcO- quant. Hydrolysis of I tri-Me ether by refluxing with N NaOH followed by the addition of Me2SO4 and boiling for 1 min. yielded the Me ester of 2,3',4,5'-tetramethoxy-6methylbiphenyl-2'-carboxylic acid, m. 124°. Demethylation yielded 2,3', 4', 5'-tetrahydroxy-6-methylbiphenyl, (II), m. 246-8°. Nitration of II after treatment at 100° in concentrated H2SO4 for 30 min. was accomplished in an ice bath with concentrated HNO3 subsequently raised to 70° to yield 2,3',4,5'tetrahydroxy-6-methyl-3,4', 5,6'-tetranitrobiphenyl-2'-sulfonic acid, (III), m. 246°. III was degraded with hypobromite in saturated Ba(OH)2. The tri-Me ether of I was oxidized with KMnO4 in N NaOH to yield 3,5-dimethoxyphthalic acid, m. 153-6°, and 4,6-dimethoxyphthalonic acid, m. 173° (decompose). The dehydration of 3,5-dimethoxyphthalic acid yielded the anhydride. m. 148-9°. Reductive decarboxylation of 4,6-dimethoxyphthalonic acid with red P and HI yielded CO2 and 3,5-dihydroxyphenylacetic acid, m. 130°, which was decarboxylated by heating the solid in a stream of N gas at 270° to yield orcinol, m. 107-8°, which sublimed. Orsellinic-carboxy-C14 acid was prepared from orsellin aldehyde-formyl-C14 (Adams and Levine, CA 17, 3867; Hoesch, CA 7, 2396). The possibility that orsellinic acid is a common precursor with other fungal phenols containing C14 skeletons is discussed.

100397-25-9, 2,3',4,5'-Biphenvltetrol, 6-methyl-

(as alternariol degradation product)

RN 100397-25-9 CAPLUS

CN [1,1'-Biphenyl]-2,3',4,5'-tetrol, 6-methyl- (CA INDEX NAME)

L34 ANSWER 28 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1961:64900 CAPLUS Full-text

DOCUMENT NUMBER: 55:64900

ORIGINAL REFERENCE NO.: 55:12349f-i,12350a-e

Hydrogen bonds. IV. Acidity and hydrogen bonds in TITLE: hydroxybiphenylenes and hydroxybiphenyl quinones

Musso, Hans; Matthies, Hans-Georg AUTHOR(S):

CORPORATE SOURCE: Univ. Gottingen, Germany Chemische Berichte (1961), 94, 356-68 SOURCE:

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal LANGUAGE: Unavailable cf. CA 54, 15322c. o,o'-Dihydroxybiphenyls showed an extraordinarily high acidity in the 1st dissociation step and a large difference in the 2nd step if a stable H bridge could form in the monoanion. If the H bridge was hindered by substituents in the 6,6'-position, the OH groups dissociated practically independently from each other. The dissociation of hydroxybiphenylquinones was investigated spectroscopically and by potentiometric titration. (o-HOC6H4)2 (18.6 g.) in 100 cc. Me2CO and 7.9 g. K2CO3 treated at reflux with stirring with 5.05 g. Me2SO4 in 20 cc. Me2CO during 40 min., the mixture refluxed 1 hr., evaporated, the residue diluted with 100 cc. H2O, acidified, extracted with Et20, the extract washed with N Na2CO3 and N NaOH, and evaporated vielded 7.62 g. o-MeOC6H4C6H4OH-o (I), m. 73-4° (50% AcOH). I (0.83 q.) in 10 cc. C5H5N-Ac2O kept 3 hrs. at room temperature gave 100% viscous oily acetate of I, b0.05 85-90°, n20D 1.5778. Phoenicin (II) (268 mq.) in 50 cc. dry CHC13 refluxed 7 min. with 250 mq. Aq20 and 5 cc. MeI, treated again with the same amts. of Ag2O and MeI, concentrated to half-volume after 12 min., filtered, washed with CHCl3, evaporated in vacuo, and the residue chromatographed on cellulose powder yielded 70 mg. unchanged II, 101 mq. mono-Me ether (III) of II.MeOH, m. 70° resolidified and rem. 139-44° (decomposition) [the melt solidified to long needles of III, m. 230-2° (decomposition)], and 79 mg, di-Me ether of III, m. 130-1° (C6H6-cyclohexane and sublimed at 110° in vacuo), followed by 61 mg. red-brown lacquer. III (30.1 mg.) heated on the microscope stage 2 hrs. at 140-5° and sublimed in vacuo gave 19.4 mg. 2,7-dimethyldibenzofuran[1,4;5,8]diquinone (anhydrophoenicin). The pK values in 50% MeOH and in H2O were determined titrimetrically and spectroscopically in both cases: PhOH, 10.78, 10.74, 9.98, 9.99; m-MeC6H4OH, -, -, -, 10.11; 2-C10H7OH, 10.56, 10.64, 9.97, -; 3,5-(HO) 2C6H3Me, 10.50, 10.66, 9.38, 9.48 (pK1) [11.96, -, 11.20, - (pK2)]; o-HOC6H4Ph, 11.22, 11.24, -, 10.01; I, 11.32, 11.42, -, 10.40; (o-HOC6H4)2, 8.00, 7.94, 7.56, 7.46 (pK1) [12.20, above 13.00, 11.80, above 13.00 (pK2)]; 3,2-(o-HOC6H4)C10H6OH, 7.94, 8.00, -, 7.55 (pK1) [11.98, above 13.00, -, above 13.00 (pK2)]; (m-HO-C6H4)2, 10.26, -, -, - (pK1) [10.90, 11.02, -, 9.86 (pK1.2)] 11.44, -, -, -(pK2); (p-HOC6H4)2, 10.40, -, -, - (pK1) [11.10, -, -, 9.62 (pK1.2); 11.70, -, -, - (pK2)]; [2,4-Me(HO)C6H3]2, 10.70, -, -, - (pK1) [11.24, -, -, 10.11 (pK1.2); 11.70, -, -, - (pK2)]; [6,2-Me(HO)C6H3]2, 11.22, -, -, -, (pK1) [11.80, 11.72, -, 10.45 (pK1.2); 12.14, -, -, -, (pK2)]; (2-HOC10H6)2, 10.64, -, -, - (pK1) [11.10, - , -, - (pK1.2); 11.68, -, -, -(pK2)]; [2,4-(HO)2C6H3]2 (IV), 7.88, -, 7.44, - (pK1) [10.75, -, 10.10, -(pK2)]; [4,2,6-Me(HO)2C6H2]2 (V), 9.04, -, 8.54, - (pK1) [9.36, -, 8.80, 8.94 (pK1.2); 9.72, -, 9.30, - (pK2); 12.03, -, 11.32, - (pK3); 12.16, -, 11.70, -(pK3.4)]; [6,2,4-Me(HO)2C6H2]2 (VI), 10.20, -, 9.34, - (pK1) [10.68, -, 9.90, 9.86 (pK1.2); 11.15, -, 10.45, - (pK2); 11.92, -, 11.45, - (pK3); 12.16, -, 11.65, - (pK3.4)]; 4,5-dihydroxy-2,7-dimethyldibenzofuran, 8.15, 7.90, -, -(pK1) [11.84, above 13.00, -, - (pK2)]; 2,7-dihydroxy-4,5dimethyldibenzofuran, 9.90, -, -, - (pK1) [10.58, -, -, - (pK1.2); 11.07, -, -, - (pK2)]; 1,8-C10H6(OH)2, 7.46, 7.42, -, 6.71 (pK1) [12.16, above 13.00, -, above 13.00 (pK2)]; o-HOC6H4CO2H, 3.74, -, 3.00 (pK1) [12.11, -, 11.70, -(pK2)]; 6-hydroxytoluquinone (VII) about 4.60, about 4.60, -, about 4.04; 3-[2,4,6-Me(HO)2C6H2] derivative (VIII) of VII, 5.38, 5.26, -, 4.37 (pK1) [10.40, 10.52, -, 9.49 (pK2)]; 6,6'-dihydroxy-3,3'-ditoludiquinone, 4.33, -, 3.93 (pK1) [4.88, 4.80, 4.28, 4.10 (pK1.2); 5.45, -, 4.79, - (pK2)]; II, 3.95, 3.85, 3.45, 3.02 (pK1) [7.30, 7.18, 6.00, 5.95 (pK2)]; III, 4.02, 4.07, -, 3.04. The infrared absorption spectrum of I, the titration curves of IV, V, and VI in 50% MeOH with 0.1N KOH in 50% MeOH, and the absorption spectra of VIII in 50% MeOH in dependence on the pH were recorded.

AB

IT 4946-96-7, 2,2',4,4'-Biphenyltetrol, 6,6'-dimethyl-(acidity of)

RN 4946-96-7 CAPLUS

KN 4946-96-/ CAPLUS

CN [1,1'-Bipheny1]-2,2',4,4'-tetrol, 6,6'-dimethy1- (CA INDEX NAME)



L34 ANSWER 29 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1958:104063 CAPLUS Full-text DOCUMENT NUMBER:

52:104063

ORIGINAL REFERENCE NO.: 52:18306b-i,18307a-b

TITLE: Orcein dyes. VII. Synthesis, constitution, and light

absorption of Henrich's quinone

AUTHOR(S): Musso, Hans

CORPORATE SOURCE: Univ. Gottingen, Germany

SOURCE: Chemische Berichte (1958), 91, 349-63

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE:

Unavailable cf. C.A. 52, 10091b; Henrich, C.A. 33, 1657. Henrich's formula suggesting that the quinone obtained by autoxidation of orcinol in aqueous KOH is 3,6,6'trihydroxy-2,2'-dimethyldiphenoquinone is improbable due to steric hindrance. The monoquinone 6-hydroxy-3-(4,6-dihydroxy-2-tolyl)toluquinone (I) has been prepared by synthesis. Successive methylation of 2-nitro-3,5-dihydroxytoluene with 3 equivs. Me2SO4 in 10% aqueous NaOH gives 2-nitro-3,5-dimethoxytoluene, m. 106°. A solution containing 1.28 g. product in 20 cc. MeOH is diluted with 45 cc. hot dilute H2SO4 and treated with Zn dust until colorless when boiled. MeOH is evaporated, dilute NaOH added, and the mixture extracted with Et20 to give 2-amino-3,5-dimethoxytoluene (II), b0.04 70°, which discolors in air. A solution of 37 mg. II in 1 cc. pyridine and 1 cc. Ac20 is left 24 hrs. and then evaporated in vacuo at 20° to yield 30.2 mg. 2-acetamido-3,5dimethoxytoluene, m. 152°. Diazotization of 0.5 g. II in 5 cc. dilute H2SO4 by dropwise addition of 0.21 g. NaNO2 in 1 cc. H2O at 0° gives the diazonium salt solution (III); after 15 min. 0.55 q. KI in 1 cc. H2O is then added, the mixture warmed 2 hrs. at 80° until N evolution is complete, and extracted with C6H6. Impurities are removed from the washed, dried solution by adsorption on Al203; evaporation yields 72% 2-iodo-3,5-dimethoxytoluene (IV), m. 84-6°. Monoiodoorcinol on methylation with Me2SO4 in aqueous NaOH at 100° and on extraction with Et20 and distillation gives orginal di-Me ether, bl 80°, and a mixture, bl 160°, separated at 10-3 mm. into IV, b. 70-80°, as well as diiodo-3,5-dimethoxytoluene (V), subliming and m. 202-3°. Direct iodination of 3.08 g. 2,4-dimethoxytoluene with 5.30 g. iodine and 4.70 g. PbO, started by adding 0.05 g. HgO and refluxing 48 hrs., is followed by chromatography of the C6H6 solution on Al203 to remove impurities and gives 2.4% V, 38% IV, and a mixture containing mono- and diiodo isomers. Deiodination of 2.52 g. IV with 7 g. electrolytic Cu in the absence of air at 100° and then for 5 hrs. at 200° is followed by extraction with C6H6 and chromatography giving 90% 4,4',6,6'tetramethoxy-2,2'-bitoly1, m. 103-4°. This product (1.87 g.) is warmed with pyridinium chloride to 150°, then at 180° for 1 hr., and finally at 200° for 0.25 hr. Extraction by Et20, alkaline extraction of the solution under N, acidification, and extraction by Et20 gives 4,4',6,6'-tetrahydroxy-2,2'bitolyl (VI), m. 237-9°, yellowing in aqueous solution and turning brown in

alkali. Treatment of the tetra-Me ether with HI gives 43% VI and 45% 2,7dihydroxy-4,5-dimethyldibenzofuran, m. 247-8°. VI with Ac20 gives the tetraacetate, m. 136-7°. Oxidation of a solution of 0.5 g. VI and 1 g. K2HPO4 in 15 cc. H2O by dropwise addition of 2 moles K nitrosodisulfonate at 0°, acidification, crystallization from the filtrate, and recrystn, from AcOH, H2O-EtOH, or CHCl3EtOH gives I, m. 131-2° (decomposition), purified by distribution chromatography. On treatment with Zn dust and Ac20, I gives 3.4,4',6,6'-pentaacetoxy-2,2-bitolyl (VII), m. 154°, also obtained by hydrogenation of the solution in Ac20 with 1.1 moles H over Pd-BaSO4, when some leucohexaacetate, m. 194-201°, is also formed. Oxidation of 0.5 g. VI with 4 moles K nitrosodisulfonate at 0° yields 4,4'-dihydroxy-2,2'bitolyldiquinone (VIII), m. 207° (discoloring from 180°), which on treatment with Zn and Ac20 gives 3,3',4,4',6,6'-hexaacetoxy-2,2'-bitoly1 (IX), m. 199-201°. Genuine Henrich's quinone is prepared, m. 155-9° (decomposition), together with some diquinone, m. 175-80° (decomposition). Reductive acetylation gives VII and IX and distribution chromatography of Henrich's quinone with BuOH-0.2M phosphate buffer at pH 7.10 on 3 cellulose columns gives I and VIII, identified by m.p. Treatment of I with o-phenylenediamine gives 3-hydroxy-1-methyl-2-(4,6-dihydroxy-2- tolyl)phenazine, m. 298-300° (acetate, m. 160° and 168°), and treatment of VIII with o-phenylenediamine gives 3,3'-dihydroxy-1,1'-dimethy1-2,2'-biphenazine, m. 220-30°(diacetate, m. 221°). Oxidation of orcinol hydrate with K nitrosodisulfonate gives 6hydroxytoluguinone, m. 117-27°, yielding 3-hydroxy-1-methylphenazine, decompose 290° (acetate, m. 149°). Resolution of a solution of I buffered to pH 9.0 by fractional chromatography on a column of starch grains of 0.05-0.075 mm. for 3 days gives $[\alpha]D20\ 153-4^{\circ}$ or $-153-4^{\circ}$ for the isomer. 4946-96-7P, 2,2',4,4'-Biphenyltetrol, 6,6'-dimethyl-114399-85-8P, 2,2',4,4'-Biphenyltetrol, 6,6'-dimethyl-, tetraacetate 124116-64-9P, 2,2',4,4',5-Biphenylpentol, 6,6'-dimethyl-, pentaacetate 124202-23-9P,

ΙT 2,2',4,4',5,5'-Biphenylhexol, 6,6'-dimethyl-, hexaacetate RL: PREP (Preparation)

(preparation of) 4946-96-7 CAPLUS

RN CN

[1,1'-Biphenvl]-2,2',4,4'-tetrol, 6,6'-dimethyl- (CA INDEX NAME)

RN 114399-85-8 CAPLUS

[1,1'-Biphenyl]-2,2',4,4'-tetrol, 6,6'-dimethyl-, 2,2',4,4'-tetraacetate CN (CA INDEX NAME)

RN 124116-64-9 CAPLUS

[1,1'-Biphenyl]-2,2',4,4',5-pentol, 6,6'-dimethyl-, CN 2,2',4,4',5-pentaacetate (CA INDEX NAME)

RN 124202-23-9 CAPLUS

CN [1,1'-Biphenyl]-2,2',4,4',5,5'-hexol, 6,6'-dimethyl-, 2,2',4,4',5,5'-hexaacetate (CA INDEX NAME)

L34 ANSWER 30 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1959:105499 CAPLUS Full-text

DOCUMENT NUMBER: 53:105499 ORIGINAL REFERENCE NO.: 53:18935b-g

TITLE: Chemistry of lichens. XI. Structure of picrolichenic

acid

AUTHOR(S): Wachtmeister, Carl A.

CORPORATE SOURCE: Kgl. Tekn. Hogskolan, Stockholm Acta Chemica Scandinavica (1958), 12, 147-64 SOURCE:

CODEN: ACHSE7; ISSN: 0904-213X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

- AB cf. C.A. 52, 12836f. Picrolichenic acid (I), prisms, m. 187-90° (decomposition) (aqueous AcOH), an intensely bitter compound isolated (5-7% yield) from the dry powdered crustose lichen Pertusaria amara, occurring on the bark of oak and beech trees, by Et20 extraction and crystallization in the cold, has been shown to have the structure (I) by decarboxylation of its piperidide [2 interconvertible forms, m. 169-72° (C6H6) and 187-9° (decomposition) (aqueous AcOH) (di-Me derivative, prisms, m. 163-5° (MeOH)] to 2,4,6-C5H11(HO)(MeO)C6H2C6H(C5H11)(CO2H)(OH)2-2,3,4,6 (II), m. 145-8° (decomposition) (C6H6). I was purified by Al2O3 treatment and recrystn. from C6H6 or aqueous AcOH; it is soluble in most common organic solvents except C6H6 and petr. ether. Brief (1 min.) treatment of I with CH2N2 in the cold gave Me picrolichenate, needles, m. 102-3.5° (MeOH), while prolonged (overnight) methylation with CH2N2gave Me O-methylpicrolichenate, needles, m. 80-2° (C6H14). Simultaneous decarboxylation and demethylation of II gives 2,2'-diamyl-4,4',6,6'-tetrahydroxybiphenyl (III), needles, m. 180-1° (glacial AcOH) (tetra-Me ether, m. 34.5-5.5° (MeOH); dibromo derivative, m. 119.5-20.5° (glacial AcOH); tribromo derivative, m. 106-7° (glacial AcOH); tetrabromo derivative, m. 97-8° (glacial AcOH)). III was identified by dehydration with ZnCl2 at 240-50° to 3,7-dihydroxy-1,9-diamyldibenzofuran (IV), m. 124-5° (C6H6petr. ether), which was methylated [di-Me ether of IV, needles, m. 72-3° (aqueous AcOH)] and oxidized by 20% KMnO4 solution to 3,7dimethoxydibenzofuran-1,9-dicarboxylic acid [di-Me ether, needles, m. 191-3.5° (EtOH)]. Infrared and ultraviolet absorption spectra further support the structures given. The unique structure of I combines features of the depsidones and of usnic acid and is comparable to the fungal metabolite griseofulvin which contains a similar spiran structure. The theory of oxidative coupling of phenols provides a common basis for a rational interpretation of the biosynthesis of dibenzofuran-like compds. from simple phenolic progenitors. 98985-63-8P, 2,2',4,4'-Biphenyltetrol, 6,6'-dipentyl-102756-33-0P, 2,4,4'-Biphenyltriol, 2'-methoxy-6,6'-dipentyl-103898-20-4P. B-Resorcylic acid.
- 102756-23-0P, 2-4,4-Baphenyltriol, 2'-methoxy-6,6'-dipentyl-102998-20-4P, B-Resorcylic acid, 5-(4-hydroxy-2-methoxy-6-pentylphenyl)-6-pentyl-RL: PREP (Preparation) (preparation of)
- RN 98985-63-8 CAPLUS
- CN [1,1'-Biphenyl]-2,2',4,4'-tetrol, 6,6'-dipentyl- (CA INDEX NAME)

- RN 102756-23-0 CAPLUS
- CN [1,1'-Biphenyl]-2,4,4'-triol, 2'-methoxy-6,6'-dipentyl- (CA INDEX NAME)

RN 102898-20-4 CAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid,

4,4',6-trihydroxy-2'-methoxy-2,6'-dipentyl- (CA INDEX NAME)

L34 ANSWER 31 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1958:6282 CAPLUS Full-text

DOCUMENT NUMBER:

: 52:6282 NCE NO.: 52:1114h-i,1115a-b

ORIGINAL REFERENCE NO.: 5

TITLE: Picrolichenic acid, a new type of lichen acid

AUTHOR(S): Erdtman, H.; Wachtmeister, C. A.

CORPORATE SOURCE: Roy. Inst. Technol., Stockholm

SOURCE: Chemistry & Industry (London, United Kingdom) (1957)

CODEN: CHINAG; ISSN: 0009-3068

DOCUMENT TYPE: LANGUAGE: Journal Unavailable

GI For diagram(s), see printed CA Issue.

AB A structure for picrolichenic acid (I), C25H3007, is proposed (cf. Zopf, Ann. 321, 32(1902). I is optically inactive and contains OH, OMe, CO, CO2H, lactone, and two C-Me groups. With CH2N2 it gives a mono-Me ester, m. 102-3.5°, and a neutral O,O-di-Me derivative, m. 80-2°. I with KMn04 gives caproic acid. In NaOH acidified in the cold it gives a gum which loses CO2 to form a monocarboxylic acid, C24H3206 (II), m. 145-8° (decomposition). II on boiling with HBr undergoes decarboxylation and demethylation to diolevitol (III), m. 180-1°. Dehydration of III with ZnCl2 gives a highly fluorescent phenol, C22H2803; the di-Me ether, m. 71.5-3°, of the latter is oxidized with permanganate to a dicarboxylic acid, the di-Me ester of which, m. 191-3.5°, is

identical with 3,7-dimethoxy-1,9-dicarbomethoxydibenzofuran (cf. Shibata, C.A. 45, 7100d). I is the first example of a lichen acid formed by intramol. C-C coupling (cf. Festschr. Arthur Stoll, Basel, 1957, p. 144; Barton and Cohen, ibid., p. 117).

IT 98985-63-8P, 2,2',4,4'-Biphenyltetrol, 6,6'-dipentyl-

RL: PREP (Preparation)

(preparation of) RN 98985-63-8 CAPLUS

[1,1'-Biphenvl]-2,2',4,4'-tetrol, 6,6'-dipentvl- (CA INDEX NAME) CN

L34 ANSWER 32 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1957:43283 CAPLUS Full-text

DOCUMENT NUMBER: 51:43283

ORIGINAL REFERENCE NO.: 51:8062c-e

TITLE: Formazyl complexes of the thiophene series AUTHOR(S): Seyhan, Muvaffak; Fernelius, W. Conrad CORPORATE SOURCE: Pennsylvania State Univ., University Park SOURCE: Chemische Berichte (1956), 89, 2482-3

CODEN: CHBEAM: ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

Diazotizing 625 mg, o-H2NC6H4CO2H in 2 cc. concentrated HCl with 375 mg, NaNO2 AB in the min. amount of H2O at -5° , adding 1 g. 2-thiophenealdehyde phenylhydrazone and 1 g. NaOH in 35 cc. MeOH at 0°, filtering off the precipitate after 4 hrs., acidifying the filtrate with AcOH, and adding H2O give 805 mg. N-phenyl-N'-(2-carboxyphenyl)-C-(2-thienyl)formazan (I), dark red crystals, m. 181-2° (decomposition). Heating 140 mg. I in concentrated aqueous solution with 90 mg. NiSO4 and NaOAc a short time on a water bath gives a Ni complex, C18H12O2N4SNi, dark green microcrystals, not m. below 320°; Cu complex, C18H12O2N4SCu, deep violet microcrystals, m. 243-4° (decomposition).

124202-23-9

(Derived from data in the 6th Collective Formula Index (1957-1961))

124202-23-9 CAPLUS RN CN

[1,1'-Biphenvl]-2,2',4,4',5,5'-hexol, 6,6'-dimethvl-,

2,2',4,4',5,5'-hexaacetate (CA INDEX NAME)

10/584,234 December 24, 2008

DOCUMENT NUMBER: 51:43284

ORIGINAL REFERENCE NO.: 51:8062e-i,8063a-f

TITLE: Rearrangements of hydroxydiquinones. I. Preparation of 2-hydroxy-4,4'-dimethyl-3,3',6,6'-diquinone and of 2,3,3',6,6'-pentahydroxy-4,4'-diphenyl

AUTHOR(S): Posternak, Th.; Alcalay, W.; Huguenin, R.

CORPORATE SOURCE: Univ. Lausanne, Switz.

SOURCE: Helvetica Chimica Acta (1956), 39, 1556-63

CODEN: HCACAV; ISSN: 0018-019X

DOCUMENT TYPE: Journal LANGUAGE: French

GI For diagram(s), see printed CA Issue.

AB cf. C.A. 38, 12186. [The nomenclature

cf. C.A. 38, 12186. [The nomenclature and numbering of the biquinones OC.CH:CR.CO.CR'':CC:CR'.CO.CR:CH.CO (A) and the (dihydroxy- or alkoxyphenyl)p-benzoquinones OC.CH:CR.CO.CR'':CC:CH.C(OR'):CR.CH:COR' (B) or their tautomeric forms OC.CH:CR.C(OR'):CR''.C:C.CH:C(OR').CR:CH.CO(B') in the original of this paper differ from C.A. usage. In this abstract the compds. are designated by A, B, or B', followed in parentheses by R, R', and R'' in that order. A mixture of 23 g. powdered A (Me, H, H) (I) and 92 g. p-C6H4(OH)2 added to 2.3 1. boiling water, boiled 1-2 min. and the air-dried product washed with boiling water yielded 20 g. B (or B') (Me, H, H) (II), m. 256-8° (corrected). AlCl3 (2.5 g.) added to 500 mg. toluguinone in 6 cc. CS2. the mixture shaken 30 min. at room temperature, and the air-dried product added portionwise to 50 cc. 2N HCl at 0° yielded 230 mg. II, m. 256-8°. II in EtOH oxidized with FeCl3 yielded I. Powdered anhydrous AlCl3 (15 g.) added to 3 g. phenyl-p-benzoquinone in 60 cc. CS2, the mixture shaken 5 hrs., the airdried product decomposed with 10% HCl at 0°, washed with boiling EtOH, and the residue recrystd. from PhNO2 yielded 1.5 g. B (or B') (Ph, H, H) (III), m. 312-15° (corrected). Powdered III (400 mg.) in 10 cc. AcOH treated with 1 cc. 6N CrO3 in AcOH, and the mixture shaken 1 hr., allowed to stand overnight, and poured into 10 cc. water yielded 370 mg. A (Ph, H, H), m. 304-9° (corrected). Powdered II (18 g.) added in 3- to 5-g. portions to 95 cc. Ac2O and 5 cc. H2SO2 at 0°, and the mixture allowed to stand 3 hrs. at room temperature and poured into 10-15 parts ice water yielded 28 g. 2,3,3',6,6'-pentaacetoxy-4,4'ditolyl (IV), m. 165-6°. IV (19 g.) refluxed 20 min. in 160 cc. N HCl under H and the product concentrated to 50 cc. and dried over KOH yielded 10.5 g. pentahydroxy analog (V) of IV, m. 220-5°. V (10 q.) in 100 cc. hot EtOH cooled, diluted with 200 cc. water, and the filtered solution added portionwise to 50 cc. 3.3N FeC13 yielded 9 g. A (Me, H, HO) (VI), m. 178-80°; acetate, m. 152-3°; Me ether, m. 102-3°. VI (1 g.) treated at 0° with 6 cc. 5% H2SO4 in Ac20, the mixture allowed to stand 24 hrs. at room temperature, poured into 10 parts ice water, the air-dried product refrigerated 24 hrs. in 2-3 parts absolute EtOH, and the insol, residue (1.3 g.) dissolved in 25 parts boiling EtOH and slowly cooled yielded 90-130 mg, rearrangement product (VII), m. 213-15°, of VI; the alc. mother liquors from VII diluted with water and the product recrystd. from AcOH yielded 400-500 mg. 1,3,4,5,6(or 8)-pentaacetoxy-2,7-dimethyldibenzofuran (VIII), m. 165°; the first two AcOH mother liquors from VIII poured into cold water yielded 170-250 mg. 2,2',3',6'-tetraacetoxy-4,4'-ditolyl-3,6-quinone (IX), m. 156°. IX (140 mg.) in 1.4 cc. Ac20 treated with 300 mg. powdered Zn and 0.3 cc. pyridine, the mixture heated to boiling until decolorized, filtered, and the filtrate poured into water yielded 150 mg. 2,2',3,3',6,6'-hexaacetoxy-4,4'-ditolyl (X), m. 202-3°. VIII (270 mg.) refluxed 30 min. with 4 cc. N HCl-MeOH, the product dried over KOH, the residue (150 mg. m. 220-5°) dissolved in 2.5 cc. hot EtOH, and the solution cooled and treated first with 2.5 cc. water, then with 0.9 cc. 2.5N FeCl3, yielded 110 mg. 3-hydroxy-2,7-dimethyldibenzofurandiquinone (XI). m. 252-4° (corrected). Powdered XI (50 mg.) dissolved in 1.5 cc. 5% H2SO4 in Ac20, and the mixture allowed to stand 48 hrs. at room temperature and poured into ice

water vielded 3,5,6,8-tetraacetoxv-2,7- dimethyldibenzofuran-1,4-quinone (XII), m. 225-35° (decomposition). XII (300 mg.) in 0.5 cc. Ac20 containing 30 mg. anhydrous NaOAc treated with 70 mg. powdered Zn, the solution filtered hot, and the combined filtrates added to cold water yielded 1,3,4,5,6,8hexaacetoxy-2,7-dimethyldibenzofuran (XIII) (hexaacetate of anhydrodihydroxyleucophenicin), m. 255-6°. VI (50 mg.) in 0.5 cc. absolute EtOH refluxed 1 hr. with 0.2 cc. cyclopentadiene and the solution evaporated vielded dicyclopentadiene-2-hydroxy-4,4'-ditoluguinone (XIV), m. 154°. B (or B') (MeO, H, H), m. 269° (corrected) (10 g.), added to 60 cc. 5% H2SO2 in Ac20 at 0° and the mixture allowed to stand 3 hrs. at room temperature yielded 200 mg. 4,4'-dimethoxydiquinone, m. 271-2° (corrected). The filtrate poured into 600 cc. ice water yielded a small amount of 3,3',6,6'-tetraacetoxy- but mostly (7.1 g.) 2,3,3',6,6'-pentaacetoxy-4,4'-dimethoxydiphenyl (XV), m. 196-7°. XV (1.08 g.) in 9 cc. N HCl-MeOH refluxed 40 min, under CO2 and the product distilled and finally dried over KOH yielded 630 mg, pentahydroxy analog (XVI) of XV, m. 194-7°. XVI with 5% H2SO4 in Ac20 vielded XV, m. 196-7°. 124202-23-9

IT 124202-23-9
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 124202-23-9 CAPLUS

CN [1,1'-Biphenyl]-2,2',4,4',5,5'-hexol, 6,6'-dimethyl-,
2,2',4,4',5,5'-hexaacetate (CA INDEX NAME)

L34 ANSWER 34 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1953:59919 CAPLUS Full-text

DOCUMENT NUMBER: 47:59919

ORIGINAL REFERENCE NO.: 47:10172e-f

TITLE: Antiseptics for foods. LV

AUTHOR(S): Fujikawa, Fukujiro; Tokuoka, Akimasa; Kometani, Eishi;

Matsubara, Shoji CORPORATE SOURCE: Kyoto Coll. Pharm.

SOURCE: Yakugaku Zasshi (1953), 73, 688-90

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

AB cf. Ca. 47, 4513c. Soy sauce with 0.01% 6-chlorothymol, p-Me2EtCC6H4OH, 2,1-HOC1OH6CHO, 3,7-dihydroxy-19-,dimethyldibenzofuran, phenothiazine, 2-methyl-1,4-naphthoquinone, and 2-ethyl-1,4-naphthoquinone prevented the growth of mold for 61 days.

4946-96-7, 4,4'-Biorcinol

(in soy-sauce preservation)

RN 4946-96-7 CAPLUS

CN [1,1'-Bipheny1]-2,2',4,4'-tetrol, 6,6'-dimethyl- (CA INDEX NAME)



L34 ANSWER 35 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1954:1175 CAPLUS Full-text DOCUMENT NUMBER: 48:1175

DOCUMENT NUMBER: 48:1175

ORIGINAL REFERENCE NO.: 48:229f-i,230a

TITLE: Antibacterial activity of some organic compounds in vitro. II. Antibacterial activity of some organic

vitro. 11. AntiDacterial activity of some organic compounds on Micrococcus pyogenes var. aureus, Escherichia coli communior, and Bacillus subtilis

AUTHOR(S): Fujikawa, Fukujiro; Hitosa, Yuhei; Yamaoka, Michiyo; Fujiwara, Yoshiko; Nakazawa, Shozo; Omatsu, Tokugoro;

Toyoda, Tadaaki

SOURCE: Yakugaku Zasshi (1953), 73, 135-8 CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

The growth-inhibitory action of the following compds. was tested on M. pyogenes var. aureus, E. coli communior, and B. subtilis, in the order named, and the effective dilns. (10,000 dilution = 1) were: (2-HOC6H4)20, 1, 1, and <1; 2-HOC6H4OC6H4OH-4, 1, 1, and <1; (4-HOC6H4)2O, 1, 1, and 1; 2-HOC6H4OC6H4Me-2, 2, 2, and 1; 2-HOC6H4OC6H4Me-4, 4, 1, and 1; 3-MeC6H4OC6H3(OH)2-2, 5, 4, 1, and 2; 2,5-(HO)2C6H3OC6H4Me-4, 2, 1, and 2; 2,5-Me2C6H3OC6H4OH-4, 8, <1, and 2; 2,4,6-Me(HO)2C6H2OC6H4Me-4, 1, <1, and <1; 2,5,3-Me2(HO)C6H2OPh, 2, 1, and 8; 2,5,3-Me2(HO)C6H2OC6H4OH-2, 1, 1, and 1; 2,5,4,6-Me2(HO)2C6HOC6H4Me-2, 2, 1, and 2; 2,5,4,6-Me2(HO)2C6HOC6H4Me-3, 1, <1, and 1; 2,5,4,6-Me2(HO)2C6HOC6H4Me-4, 1, <1, and 1; 2-HO2CC6H4OPh, 1, 1, and <1; 3-H02CC6H4OPh, all <1; 2-H0C6H4CC6H4CO2H-2, all <1; 3-H0C6H4CC6H4CO2H-3, 1, 1, and <1; 3-HO2CC6H4OC6H4OH-4, all <1; 3-HO2CC6H4OC6H4OMe-4, all <1; PhOC6H3(OH)CO2H-3,5, all <1; 2-HO2CC6H4CC6H4CO2H-4, all <1; 3,5-HO(HO2C)C6H3OC6H4CO2H-4, all <1; 4-ClC6H4OC6H4OMe-4, all 1; 4-ClC6H4OC6H4OH-4, all 1; (2-HOC6H4)2, all 1; [2,4-(HO)2C6H3]2, 1, 1, and <1; [2,4,6-Me(MeO)2C6H2]2, all <1; [2,4,6-Me(HO)2C6H2]2, 2, 1, and <1; [2,4,5-(HO) 2RC6H212, R = cyclohexyl, 1, <1, and 1; (4-HO2CC6H4)2, all <1; [2,5,4,6-Me2(HO)2C6H]2, all <1; 2,7-dimethoxy-4,5-dimethyldiphenylene oxide, all <8; 2,7-dihydroxy-4,5-dimethyldiphenylene oxide, <8, <8, and 16; 2,7dihydroxydiphenylene oxide 4.5-dicarboxylic acid, all <8; the Me ester of the latter, all <8; divaricatic acid, 2, <1, and 16; atranorin, <1, 1, and <1; sekikaic acid, 1, <1, and 4; sphaerophorin, 1, <1, and 16; gyophoric acid, all <8; anziaic acid, all 8; microphyllic acid, all 8; Me lecanorate, all <1; protocetraric acid, all 8; α -collatolic acid, all 8; β -collatolic acid, <8, 8, and <8; collatolon, 16, 8, and <8; stictinic acid, <8, 8, and <8; psoromic acid, all <1; usnolic acid, all <1; Et usnolate, 2, 4, and 4; usnetol, all <1; rangiformic acid, 8, 8, and <8; 1-protolichesterinic acid, 8, <1 and 1; agaricinic acid, 1, 1, and <1; sphaerophorol, 8, 1, and 8. 4946-96-7, 2,2',4,4'-Biphenyltetrol, 6,6'-dimethyl-

(antibacterial effects of)

RN 4946-96-7 CAPLUS

CN [1,1'-Bipheny1]-2,2',4,4'-tetrol, 6,6'-dimethyl- (CA INDEX NAME)



L34 ANSWER 36 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1952:61282 CAPLUS Full-text

DOCUMENT NUMBER: 46:61282 ORIGINAL REFERENCE NO.: 46:10286g-i,10287a

TITLE: Effect of some compounds on the tubercle bacilli in

vitro. IV

AUTHOR(S): Naito, Masakazu; Shihoda, Akira; Ohta, Masahisa;

Fujikawa, Fukujiro; Nakajima, Kunio; Fujii, Hiroshi; Tokuoka, Akimasa; Hitosa, Yuhei

SOURCE: Yakugaku Zasshi (1952), 72, 1047-50 CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal Unavailable

LANGUAGE:

cf. C.A. 46, 4052b. Growth inhibition of Mycobacterium tuberculosis in vitro by the following compds. was tested: phenanthrenequinone (I) and its 9,10-[:NNHC(:NH)NH2.HNO3]2, thymoguinone (II), its 5-[:NNHC(:NH)NH2.HNO3] (III) and 2,5-[:NNHC(:NH)NH2.HNO3]2, toluguinone and its mono- and bis-

aminoquanylhydrazone-HNO3, p-benzoquinone (IV) and its

monoaminoquanylhydrazone (V) and its mono- and bis-aminoquanylhydrazone-HNO3, 1,4-naphthoquinone (VI), its mono- (VII) and bisaminoguanylhydrazone-HNO3, 2methyl-1,4-naphthoquinone (VIII), its mono- and bisamino-guanylhydrazone-HNO3, anthraquinone, 2-methylanthraquinone (IX), 2-methyl-5-methoxy-1,4-

benzoquinone, 2,7-dihydroxy-4,5-dicarboxydiphenylene dioxide, 2,7-dihydroxy-1,4,5,8-tetramethyldiphenylene dioxide, 2,7-dihydroxy-4,5-dimethyldiphenylene dioxide, 6,6'-dimethyl-2,2',4,4'-tetra-hydroxybiphenyl, and p-

H2NO2SC6H4CH:NNHCSNH2 (X); 2,4-H0(H2N)C6H3CO2Na (XI) is used as a control. Compds. I to XI, inclusive, inhibited the growth at the dilution of 1: 160,000; II, VI, VIII and XI were effective at the dilution of 1:320,000. Of

42 lichen compds. tested, none showed remarkable growth inhibition except that Me evernate was effective at 1:80,000, while atranorin, Me and Pr lecanaorate, and iso-Bu and Am evernate were effective at 1:40,000. 2,4-HO(H2N)C5H3CO2Ph was effective at 1:600,000-1:640,000.

4946-96-7, 2,2',4,4'-Biphenvltetrol, 6,6'-dimethyl-

(effect on tubercle bacilli)

4946-96-7 CAPLUS RN

CN [1,1'-Biphenyl]-2,2',4,4'-tetrol, 6,6'-dimethyl- (CA INDEX NAME)



L34 ANSWER 37 OF 39 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1951:39034 CAPLUS Full-text

DOCUMENT NUMBER: 45:39034 ORIGINAL REFERENCE NO.: 45:6692b-d

Antibacterial effects of lichen substances. II. TITLE:

Antibacterial effects of didymic acid and its related

compounds

AUTHOR(S): Shibata, Shoji; Miura, Yoshiaki; Sugimura, Hisako; Toyoizumi, Yuri

CORPORATE SOURCE:

Univ. Tokyo SOURCE:

Yakugaku Zasshi (1948), 68, 303-5 CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

Antibacterial effects of didymic acid and strepsilin of the dibenzofuran group of lichen substances and their derivs. were examined The antibacterial power of didymic acid is controlled by its dibenzofuran ring, its OH group, and the number of C atoms in its alkyl group. The strongest antibacterial power in lichen substances and their derivs. was shown by decarboxynordidymic acid (I). The highest dilns, inhibiting growth of M. tuberculosis (avian type) and Staph. aureus, resp., were: strepsilin < 1:10,000, < 1:5,000; didymic acid 1:40,000, 1:80,000; I 1:320,000, 1:640,000; diacetate of I -, < 1:5,000; 1,9dimethy1-3,7-dihydroxydibenzofuran 1:80,000, 1:80,000; 1-methy1-3,7dihydroxydibenzofuran -, 1:40,000; 3,7-dihydroxydibenzofuran 1:10,000, 1:5,000; 1,4,6,9-tetramethyl-3,7-dihydroxydibenzofuran <1:10,000, <1:5,000; dibenzofuran -, < 1:5,000; 1,9-dimethyl-3,7-dimethoxydibenzofuran -, < 1:5,000; 6,6'-dimethyl-2,2',4,4'-tetrahydroxybiphenyl -, 1:5,000; orcinol -, < 1:5,000; olivetol 1:10,000, 1:10,000; sphaerophorol 1:40,000, 1:40,000.

ΙT 4946-96-7, 2,2',4,4'-Biphenyltetrol, 6,6'-dimethyl-

(antibacterial effects of)

4946-96-7 CAPLUS RN CN

[1,1'-Biphenyl]-2,2',4,4'-tetrol, 6,6'-dimethyl- (CA INDEX NAME)

10/584.234 December 24, 2008

ACCESSION NUMBER: 1951:41441 CAPLUS Full-text

DOCUMENT NUMBER: 45:41441

ORIGINAL REFERENCE NO.: 45:7100d-i,7101a-d

TITLE: Didymic acid, a new kind of lichen substance Shibata, Shoji AUTHOR(S):

CORPORATE SOURCE: Imperial Univ., Tokyo

Acta Phytochimica (1944), 14, 9-38 SOURCE: CODEN: APCJA8; ISSN: 0365-5393

DOCUMENT TYPE:

AB

Journal LANGUAGE: German

> Concentration of the Et20 extract of 1500 g. of a mixture of Cladonia species vielded, successively, 1.5 g. squamatic acid, 2 g. barbat(in)ic acid, and 1.7 g. didymic acid (I). I, C22H26O5, recrystd. from petr. ether, m. 172-3° (decomposition), develops colors as follows: FeCl3, blue; CaCl2 on crystals moist with EtOH, blue-green; concentrated H2SO4, yellow to green on warming. It is readily soluble in aqueous NaOH, EtOH, Et2O, and Me2CO, difficultly soluble in aqueous Na2CO3 or NaHCO3, AcOH, C6H6, or petr. ether. With Ac2O and C5H5N, it yields I acetate, colorless needles, m. 116°. With CH2N2 in Et2O, it gives colorless prisms, m. 109°. I (100 mg.), melted at 200° and vacuumdistilled at 0.015 mm. Hg and 210-50°, gave 50 mg. decarboxydidymic acid (II), m. 81-2° (petr. ether), gives no color with FeCl3 and a blue-green color with CaCl2-EtOH, is soluble in most organic solvents. II (47 mg.), refluxed 2 h. with 2 mL. HI and 1 mL. AcOH, the solution poured into ice H2O, and the precipitate filtered and recrystd. from petr. ether-C6H6, gave 10 mg. decarboxynordidymic acid (III), m. 120°. III (20 mg.) kept overnight in 0.5 mL. C5H5N and 1 mL. Ac2O, precipitated in H2O, and recrystd. from dilute aqueous EtOH, colorless needles, m. 60-1°, soluble in C6H6, EtOH, and petr. ether. I (200 mg.) was added in portions to 6 g. KOH, 0.4 g. Zn dust, and 4 drops H2O, the temperature raised from 160 to 250° in 15 min., held 10 min. at 250-70° and 5 min. at 270-310°, the melt dissolved in H2O, acidified with HCl, extracted with Et20, the Et20 extract shaken with aqueous Na2CO3, taken to dryness, and the residue recrystd. from H2O, giving 10 mg. C20H26O4, m. 155-6°, soluble in aqueous NaOH (red solution), EtOH, Et2O, and Me2CO, less soluble in hot H2O and C6H6. 3,5-(MeO)2C6H3Pr (IV) (1.5 g.) (C.A. 30, 6351.9) and 2.1 g. iodine in 50 mL. Et2O, treated with 1.5 g. HgO, shaken 7 h. for complete decolorization, filtered, washed with NaHSO3, KI, and KOH solns., and evaporated gave 0.9 g. 2,3,5-I(MeO)2C6H2Pr (V), oil, b8 150-60°. V (1 g.) and 2.5 g. Cu powder, heated 5 h. at 210-20° in a sealed tube, extracted with hot Me2CO, and the Me2CO-free residue distilled, gave 0.2 g. IV, b4 140-60°, and 0.1 g. 2,2'-dipropyl-4,4',6,6'-tetramethoxybiphenyl (VI), b0.06-0.08 200-10°. VI (0.1 g.) was demethylated with HI to 2,2'-dipropyl-4,4',6,6'tetrahydroxybiphenyl, easily soluble in EtOH, gives no color with FeCl3 and a fugitive violet-red color with CaCl2-EtOH. 2,2'-Dimethyl-4,4',6,6'tetramethoxybiphenyl (VII) (8 q.), heated 6 h. on an oil bath with 58 mL. HI and a little red P, gave 2 g. 4,5-dimethyl-2,7-dihydroxydibenzofuran (VIII) and 4.5 g. 2,2'-dimethyl-4,4',6,6'-tetrahydroxybiphenyl, yellow leaflets from PhNO2, m. 232-3°. VII (4 g.) heated 4 h. on an oil bath with 75 mL. HI gave only VIII, colorless leaflets, m. 243°, soluble in Et20 and Me2CO, insol. in H2O. VIII (3.5 g.), refluxed 5 h. with 10 mL. Me2SO4 in 50 mL. Me2CO and 20 q. K2CO3, gave 2.6 g. 4,5-dimethyl-2,7-dimethoxydibenzofuran (IX), colorless leaflets, m. 157°, gives no color with FeCl3 and CaCl2. IX (0.1 g.) in 10 mL. C5H5N, treated 6 h. with 0.25 g. KMnO4 in 10 mL. H2O on a boiling water bath, gave 0.05 g. 5-methyl-2,7-dimethoxy-4-dibenzofurancarboxylic acid, colorless needles, m. 181°, easily soluble in EtOH (blue fluorescence). IX (0.3 g.) in 10 mL. C5H5N, treated 15 h. with 3 g. KMnO4 in 75 mL. H2O on a boiling water bath, gave 0.07 g. 2,7-dimethoxy-4,5-dibenzofurandicarboxylic acid (X), m. 321-2° (decomposition) (from p-dioxane), readily soluble in EtOH, less soluble in Et20, shows intense blue fluorescence. X with CH2N2 gave X di-Me ester,

vellowish prisms, m. 188.5-9.5° (from EtOH), readily soluble in Et2O, shows blue fluorescence. II (0.11 g.), refluxed 3 h. in 40 mL. Me2CO with 4 g. K2CO3 and 2 mL. Me2SO4, gave decarboxydidymic acid Me ether (XI), m. 31°. XI treated 13 h. in C5H5N on a water bath with aqueous KMnO4 gave 0.02 g. vellow needles, m. 323° (decomposition) (from p-dioxane), mixed m.p. with authentic X, 322° (decomposition). The mixed m.ps. of X di-Me esters was also not depressed. I Me ether Me ester, m. 109° (0.1 q.), in 5 mL. C5H5N, refluxed 5 h. with 0.8 g. KMnO4 in 20 mL. H2O, gave 0.02 g. vellow needles, m. 136° (from dilute p-dioxane) of 5-propyl-2,7-dimethoxy-3,4-dibenzofurandicarboxylic acid 3-mono-Me ester (XII), readily soluble in EtOH, Me2CO, Et2O, and p-dioxane, less soluble in petr. ether, shows no fluorescence. Saponification of XII and recrystn. of the product from petr. ether-p-dioxane gave the free dicarboxylic acid, m. 209-10° (decomposition), readily soluble in p-dioxane and EtOH, difficultly soluble in petr. ether and H2O. XII and CH2N2 gave di-Me ester, yellow prisms, m. 130-1° (from petr. ether). Didymic acid is 4-amyl-5-propyl-2-hvdroxv-7-methoxv-3-dibenzofurancarboxvlic acid.

4946-96-7P, 2,2',4,4'-Biphenyltetrol, 6,6'-dimethyl-ΙT 854243-85-9P, 2,2',4,4'-Biphenvltetrol, 6,6'-dipropvl-RL: PREP (Preparation)

(preparation of) RN 4946-96-7 CAPLUS

CN [1,1'-Biphenvl]-2,2',4,4'-tetrol, 6,6'-dimethyl- (CA INDEX NAME)

RN 854243-85-9 CAPLUS

[1,1'-Biphenv1]-2,2',4,4'-tetrol, 6,6'-dipropv1- (CA INDEX NAME)

L34 ANSWER 39 OF 39 WPIX COPYRIGHT 2008 ACCESSION NUMBER: DOC. NO. CPT.

TITLE:

2005-522497 [53] WPIX C2005-158513 [53]

B05

Heat shock protein-90 inhibitor for treating e.g. malignant tumors, contains benzene derivative, or its prodrug or salt, as active ingredient

THOMSON REUTERS on STN

DERWENT CLASS:

10/584,234 December 24, 2008

INVENTOR: KAJITA J; KANDA Y; KITAMURA Y; NAKAGAWA H; NAKASHIMA T;

NAKATSU R; NARA S; SHIOTSU Y; SOGA S; KITAMURA Y H K;

NAKATSU R H K

PATENT ASSIGNEE: (KYOW-C) KYOWA HAKKO KOGYO KK

COUNTRY COUNT: 107

PATENT INFO ABBR.:

PAT	TENT NO	KINI	DATE	WEEK	LA	PG	MAIN	IPC
WO	2005063222	A1	20050714	(200553)*	JA	311[1]		
EP	1704856	A1	20060927	(200663)	EN			
US	20070155813	A1	20070705	(200746)	EN			
JP	2005516721	Х	20070719	(200749)	JA	275		

APPLICATION DETAILS:

PATENT NO KIND	APPLICATION DATE
WO 2005063222 A1	WO 2004-JP19742 20041224
EP 1704856 A1	EP 2004-808092 20041224
EP 1704856 A1	WO 2004-JP19742 20041224
US 20070155813 A1	WO 2004-JP19742 20041224
US 20070155813 A1	US 2006-584234 20060626
JP 2005516721 X	WO 2004-JP19742 20041224
JP 2005516721 X	JP 2005-516721 20041224

FILING DETAILS:

PAT	TENT NO	KIND			PA:	TENT NO	
EP	1704856	A1	Based	on	WO	2005063222	Α
JP	2005516721	X	Based	on	WO	2005063222	A

PRIORITY APPLN. INFO: JP 2003-432776 20031226

AN 2005-522497 [53] WPIX

AB WO 2005063222 A1 UPAB: 20051223

NOVELTY - Heat shock protein-90 (Hsp90) inhibitor contains a benzene derivative (I), or its prodrug or salt, as an active ingredient.

DETAILED DESCRIPTION - A heat shock protein-90 (Hsp90) inhibitor contains a benzene derivative of formula (I), or its prodrug or salt, as an active ingredient.

n = 0-10;

R1 = H, OH, CN, COOH, nitro, halo, optionally substituted lower alkyl, lower alkenyl, lower alkynyl, cycloalkyl, lower alkoxycarbonyl, aroyl, lower alkanoyl, heterocyclic alkyl, aryl, aralkyl, arylsulfonyl, heterocyclyl, -CONR7R8, -NR9R10 or -OR13;

R7 and R8 = H, optionally substituted lower alkyl, cycloalkyl, lower alkanoyl, aryl, heterocyclic alkyl or aroyl, or R7 and R8 form optionally substituted heterocycly with adjacent nitrogen atom.

R9 and R10 = H, optionally substituted lower-alkyl sulfonyl, lower alkyl, cycloalkyl, lower alkanoyl, aryl, heterocyclyl, aralkyl, heterocyclic alkyl, aroyl or -CONR11R12, or R9 and R10 combine with adjacent nitrogen atom to form heterocyclyl;

R11 and R12 = as R7;

R13 = optionally substituted lower alkyl, lower alkenyl, lower alkanovl, aryl, heterocyclyl, aralkyl or heterocyclic alkyl;

 $\mbox{R2} = \mbox{optionally substituted lower alkyl, lower alkenyl, lower alkynyl, aryl or heterocyclyl (excluding optionally substituted pyrazolyl);}$

- R3 and R5 = H, optionally substituted lower alkyl, lower alkenyl, lower alkanoyl, cycloalkyl, lower-alkyl sulfonyl, arylsulfonyl, mono/di-lower-alkyl aminocarbonyl, lower alkoxycarbonyl, heterocyclic carbonyl, aralkyl or aroyl, carbamoyl; and
- R4 and R6 = H, OH, halo, CN, nitro, optionally substituted lower alkyl, lower alkenyl, lower alkynyl, lower alkoxy, cycloalkyl, lower alkoxycarbonyl, aryloxy, aryl, heterocyclyl (excluding optionally substituted pyrazolyl), lower alkanoyl, aralkyl or heterocyclic alkyl, or amino, mono/di-lower alkyl amino or COOH.

INDEPENDENT CLAIMS are also included for the following:

- (A) a benzene derivative of formula (IA) or its salt;
- (B) a pharmaceutical containing the benzene derivative (IA) or its salt as an active ingredient;
- (C) a Hsp90 inhibitor containing the benzene derivative (IA) or its salt as an active ingredient;
- (D) a therapeutic agent of disease accompanied by Hsp90 using the benzene derivative (IA) or its salt as an active ingredient;
- (E) an antitumor agent containing the benzene derivative (IA) or its salt as an active ingredient;
- (F) inhibition of Hsp90 by administering the benzene derivative or(IA), its prodrug or salt; and
- (G) use of the benzene derivative (I) or (IA), its prodrug or salt for the manufacture of the inhibitor or antitumor agent.
- R2A = optionally substituted aryl or aromatic heterocyclyl (excluding optionally substituted pyrazolyl);
- R3A and R5A = H, carbamoyl, sulfamoyl optionally substituted lower alkyl, lower alkenyl, lower alkanoyl, lower-alkyl sulfonyl, mono/di-lower alkyl aminocarbonyl, lower alkoxycarbonyl, heterocyclic carbonyl, aralkyl or aroyl;

R4A = H, OH or halo; and

- nA = 0-5.
- (1) When nA is 0, RlA is H, CH3, OH, OCH3, COOH, methoxycarbonyl, carbamoyl, -CONHCH3, -CONHCH3, -CON(CH3)Eh, propionyl, benzoyl, dioxolanyl, optionally substituted vinyl or propa-1-en-1-yl (where Ph is phenyl). When RlA is H, R6A is optionally substituted lower alkyl. When RlA is CH3, OH, OCH3, COOM, methoxycarbonyl, carbamoyl, -CONHCH3, -CON(CH3)2, -CONHCH2h, -CONHCH3, -CONHCH3, -CONHCH2h, bropionyl, benzoyl, dioxolanyl, optionally substituted vinyl or propa-1-en-1-yl, R6A is halo.
- (2) When nA is 1-5, R1A is OH, CN, COOH, halo, optionally substituted lower alkyl, lower alkenyl, lower alkynyl, cycloalkyl, lower alkanoyl, lower alkoxycarbonyl, aryl, aroyl, heterocyclic alkyl, aralkyl, arylsulfonyl or heterocyclyl, -CONR' R8, -MRSR10 or -OR13, R6A is H, halo, CN, nitro, amino, mono/di-lower alkyl amino, COOH, optionally substituted lower alkyl, lower alkenyl, lower alkoxy, cycloalkyl, lower alkanoyl, lower alkoxycarbonyl, aryloxy, aryl, heterocyclyl (excluding optionally substituted pyrazolyl), aralkyl or heterocyclic alkyl.
 - (a) When R3A and R5A are isopropyl, R6A is not H.
- (b) When R3A and R5A are methyl, R6A is not H, Br, ethyl, 1hydroxyethyl, 1-(dimethylamino)ethyl, vinyl or COOH.
- (c) When R4A and R6A are H, and R3A and R5A are tert-butyl or benzyl, (CH2)nAR1A is not the group chosen from hydroxymethyl and 2-chloro allyl.
- (d) When R4A and R6A are H, R3A is benzyl or acetyl and R5A is methyl, or when R3A, R4A and R6A are H and R5A is CH3, -(CH2)nARIA is not 2-(acetyl amino) propyl and 2-(substitution lower alkanovl amino) propyl.
- (e) When R3A-R5A are H and R6A is COOH, or when R4A, R5A and R6A are H and R3A is CH3, $-(CH2)\,nAR1A$ is not n-pentyl.
- (f) When R3A and R4A are H, and R5A is CH3 and R6A is ethyl, (CH2)nAR1A is not n-propyl.
- (g) When R3A is CH3, R4A and R6A are H and R5A is 4-methoxy benzyl, (CH2)nAR1A is not -(CH2)3CH=CH2 and -(CH2)5CH=CH2.

(h) When R3A-R6A are H and -(CH2)nARIA is (1) n-pentyl, R2A is not 2,4-dihydroxy-6-pentylphenyl, (2) n-hexyl, R2A is not 4,6-di(substituted phenyl)triazole-2-yl or 3,6-di (substituted phenyl)-1,2,4-triazine-5-yl, or (3) n-heptyl, R2A is not a substituted triazolyl.

(i) When R3A is H or acetyl, R5A is methyl, and R4A and R6A are H and - (CH2)nARIA is ethyl or 11-propyl, R2A is not 2-amino pyrimidine-4-yl which has a substituent in 5-th position.

(j) R3A-R5A are H, when R6A is OCH3 and -(CH2)nAR1A is 3-methyl picryl-en-l-yl or 3-hydroxy-3- methylbutyl, R2A is not 7-hydroxy-4-oxo-4H-l-benzopyran-3-yl or 6-methoxy-2.2-dimethyl-2H-l-benzopyran-8-yl

ACTIVITY - Cytostatic.

Human breast cancer derived KPL-4 cell proliferation inhibiting effect of 3,5-dihydroxy -2-phenyl methyl phenyl acetate (Ia) was evaluated. (Ia) showed 50% cell growth inhibition activity (GI50) of 50 micronsol or less.

MECHANISM OF ACTION - HSP-Antagonist-90.

Human N terminal recombinant Hsp90 protein was prepared according to method specified in (Cell), 89, 239-250 (1997). 3,5-dihydroxy -2-phenyl methyl phenyl acetate showed 30% or more binding with Hsp90 protein of biotinated Radicicol at concentration of 10 micronsol or less and inhibited Hsp90.

USE - For treating diseases (accompanied by Hsp90 protein) e.g. malignant tumors (claimed), hematopoietic tumors (lymphomas), solid tumors

(e.g. breast cancer), leukemia and multiple myeloma. ADVANTAGE - The benzene derivative effectively inhibits Hsp protein and provides excellent antitumor effect.

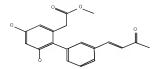
AN.S DCR-1110308

CN.S (4,6-Dihydroxy-biphenyl-2-yl)-acetic acid methyl ester

SDCN RAIKDK

AN.S DCR-1110309

SDON RATEDI.



 $\hbox{CN.S } (4,6-\hbox{Dihydroxy-3-morpholin-}4-yl\text{methyl-biphenyl-}2-yl)-acetic acid methylester \\$

SDCN RAIKDM

AN.S DCR-1110311

CN.S 2-(3-Bromo-4,6-dihydroxy-biphenyl-2-yl)-N-pyridin-3-ylmethyl-acetamide SDCN RAIKDN

CN.S N-(1-Benzyl-piperidin-4-yl)-2-(3-bromo-4,6-dihydroxy-biphenyl-2-yl)-acetamide

SDCN RAIKDO

AN.S DCR-1110313

CN.S 2-(3-Bromo-4,6-dihydroxy-biphenyl-2-y1)-N-(2,4-dimethoxy-benzyl)-acetamide SDCN RAIKDP

AN.S DCR-1110314

CN.S 5-Bromo-6-(tetrahydro-furan-2-ylmethoxymethyl)-biphenyl-2,4-diol

SDCN RAIKDQ

CN.S 2-(3-Bromo-4,6-dihydroxy-biphenyl-2-yl)-1-[4-(2-methoxy-phenyl)-piperazin-1-yl]-ethanone

SDCN RAIKDR

AN.S DCR-1110316

CN.S 6-[2-(2,3-Dihydroxy-propoxy)-ethyl]-5-ethyl-3'-(2-methyl-thiazol-4ylmethoxy)-biphenyl-2,4-diol

SDCN RAIKDS

10/584,234

AN.S DCR-1110317
CN.S 5-[2-(3-Ethyl-4,6-dihydroxy-biphenyl-2-yl)-ethyl]-oxazole-4-carboxylic acid bis-(2-hydroxy-ethyl)-amide
SDCN RAIKDT

AN.S DCR-1110318

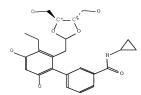
CN.S 6-((48,55)-4,5-Bis-hydroxymethyl-1,3-dioxolan-2-ylmethyl)-5-ethyl-biphenyl-2,4-dio16-((48,55)-4,5-Bis-hydroxymethyl-[1,3]dioxolan-2-ylmethyl)-5-ethylbiphenyl-2,4-dio1

SDCN RAIKDU

AN.S DCR-1110319

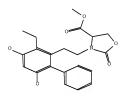
CN.S 2'-((45,55)-4,5-Bis-hydroxymethyl-1,3-dioxolan-2-ylmethyl)-3'-ethyl-4',6'-dihydroxy-biphenyl-3-carboxylic acid cyclopropylamide2'-((45,55)-4,5-Bis-hydroxymethyl-[1,3]dioxolan-2-ylmethyl)-3'-ethyl-4',6'-dihydroxy-biphenyl-3-carboxylic acid cyclopropylamid

SDCN RAIKDV



CN.S 3-[2-(3-Ethyl-4,6-dihydroxy-biphenyl-2-yl)-ethyl]-2-oxo-oxazolidine-4carboxylic acid methyl ester

SDCN RAIKDW



AN.S DCR-1110322

CN.S (3-Benzyl-4,6-dihydroxy-biphenyl-2-yl)-acetic acid methyl ester

SDCN RAIKDY

10/584,234 December 24, 2008

=> d his nofil (FILE 'HOME' ENTERED AT 11:11:09 ON 24 DEC 2008) FILE 'REGISTRY' ENTERED AT 11:11:16 ON 24 DEC 2008 L1 STR 5 SEA SSS SAM L1 L2 869 SEA SSS FUL L1 L3 SAVE TEMP L3 NIZAL234/A FILE 'CAPLUS' ENTERED AT 11:18:56 ON 24 DEC 2008 L4 357 SEA SPE=ON ABB=ON PLU=ON L3 1.5 2 SEA SPE=ON ABB=ON PLU=ON US200!-584234/APPS L6 1 SEA SPE=ON ABB=ON PLU=ON L4 AND L5 D SCA TI D SCA TI L5 FILE 'REGISTRY' ENTERED AT 11:19:30 ON 24 DEC 2008 L7 STR L1 L8 1 SEA SUB=L3 SSS SAM L7 D SCA 15 SEA SUB=L3 SSS FUL L7 L9 FILE 'CAPLUS' ENTERED AT 11:25:21 ON 24 DEC 2008 L10 2 SEA SPE=ON ABB=ON PLU=ON L9 L11 1 SEA SPE=ON ABB=ON PLU=ON L10 AND L5 FILE 'STNGUIDE' ENTERED AT 11:26:25 ON 24 DEC 2008 FILE 'REGISTRY' ENTERED AT 11:40:14 ON 24 DEC 2008 L12 STR L1 L13 10 SEA SUB=L3 SSS SAM L12 L14 322 SEA SUB=L3 SSS FUL L12 D OUE FILE 'CAPLUS' ENTERED AT 12:07:22 ON 24 DEC 2008 L15 39 SEA SPE=ON ABB=ON PLU=ON L14 L16 1 SEA SPE=ON ABB=ON PLU=ON L15 AND L6 L17 1 SEA SPE=ON ABB=ON PLU=ON L10 AND L15 L18 2 SEA SPE=ON ABB=ON PLU=ON L17 OR L10 L19 38 SEA SPE=ON ABB=ON PLU=ON L15 NOT L18 FILE 'WPIX' ENTERED AT 12:08:43 ON 24 DEC 2008 1.20 0 SEA SSS SAM L7 L21 0 SEA SSS FUL L7 L22 1 SEA SSS SAM L12 L23 17 SEA SSS FUL L12 L24 3 SEA SPE=ON ABB=ON PLU=ON L23/DCR FILE 'BEILSTEIN' ENTERED AT 12:09:51 ON 24 DEC 2008 L25 0 SEA SSS SAM L7 L26 0 SEA SSS FUL L7 L27 3 SEA SSS SAM L12 L*** DEL 1 S L2 FUL 39 SEA SSS FUL L12 39 SEA SSS FUL L12 18 SEA SPE=ON ABB=ON PLU=ON L28 AND RN/FA

10/584,234 December 24, 2008

	10.	/584,234
L30 L31	21 SEA SPE=ON ABB=ON PLU= 5 SEA SPE=ON ABB=ON PLU=	
L32 L33	FILE 'MARPAT' ENTERED AT 12:11:17 C 50 SEA SSS SAM L7 14 SEA CSS SAM L7	ON 24 DEC 2008
	FILE 'CAPLUS' ENTERED AT 12:21:07 (D QUE L18 D L18 IBIB ABS HITSTR TO D QUE L19	
	FILE 'WPIX' ENTERED AT 12:21:49 ON D QUE L24	24 DEC 2008
L34	FILE 'CAPLUS, WPIX' ENTERED AT 12:2 39 DUP REM L19 L24 (2 DUPL) ANSWERS '1-38' FROM FI ANSWER '39' FROM FI D L34 IBIB ABS HITSTR TC	(CATES REMOVED) M FILE CAPLUS (LE WPIX